

## **Transport consistent diffusion coefficient for CMFD acceleration and comparison of convergence properties**

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A diffusion coefficient for the coarse mesh finite difference (CMFD) acceleration is derived from the semi-analytic solution of one-group, one-dimensional, even-parity transport equation. The derived diffusion coefficient, *i.e.*, the transport consistent diffusion coefficient (TCD), depends on the optical length of a mesh and shows similar behavior with the artificial grid diffusion (AGD) and the effective diffusion (EffD) coefficients for an optically thick mesh. Convergence properties of typical diffusion coefficients are evaluated using the linearized Fourier analysis. Analyses of the C5G7 3D benchmark problems with and without voided region are carried out to compare the convergence properties. The number of transport sweeps to reach convergence using TCD is smaller than that using EffD or AGD.

***Keywords; CMFD acceleration, MOC, convergence, even-parity transport equation, linearized Fourier analysis, C5G7 benchmark problem***

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## 1 **1. Introduction**

2           The CMFD and the generalized coarse mesh rebalance (GCMR) acceleration methods  
3 are widely used for convergent acceleration of transport calculation based on the method of  
4 characteristics (MOC) [1]–[9]. The original idea of the CMFD method was developed by Smith  
5 for the acceleration of the advanced nodal method [1]. Later, it has been applied to various  
6 neutronics analysis codes due to its efficiency with improvements and generalizations [2]–[9].  
7 The CMFD and GCMR methods utilize the finite difference approximation based on the  
8 diffusion theory. Thus, the acceleration scheme depends on the diffusion coefficient used in the  
9 finite-difference approximation. It is well known that the CMFD and the GCMR methods show  
10 instability for a thick and diffusive mesh. In more detail, these non-linear acceleration methods  
11 generally show instability when the optical thickness of a mesh exceeds 1.0 when conventional  
12 diffusion coefficient is used [4].

13           Various stabilization methods have been proposed and implemented, *e.g.*, increasing  
14 the number of transport sweeps between CMFD accelerations, application of a damping factor,  
15 corrections on a diffusion coefficient [10]. Among them, the present study focuses on the  
16 correction of diffusion coefficient.

17           Larsen et al. proposed the effective diffusion (EffD) coefficient to preserve the net  
18 current obtained by the step characteristics transport solution using the spatially discretized  
19 transport solution with the weighted diamond-difference scheme [11]. Jarrett et al. introduced  
20 the artificial grid diffusion (AGD) coefficient to make the CMFD acceleration and the partial  
21 current based CMFD (pCMFD) acceleration [12] equivalent [10]. The EffD and the AGD  
22 coefficients make the CMFD and GCMR acceleration stable [13]. The EffD and AGD  
23 coefficients are larger than the conventional diffusion coefficients. Stabilization of  
24 CMFD/GCMR acceleration with artificially increased diffusion coefficient is also pointed out  
25 by one of the authors [4].

26           In this paper, the transport consistent diffusion (TCD) coefficient that preserves the

1 semi-analytic solution of the one-group, one-dimensional, even-parity transport equation is  
2 derived. The two-node problem, which is commonly used in the CMFD acceleration method  
3 for the advance nodal method, is used for derivation. The even-parity transport equation is used  
4 for derivation due to its similarity with the diffusion equation.

5 In section 2, derivation of the transport consistent diffusion coefficient and convergence  
6 analysis methodology of the CMFD acceleration using the linearized Fourier analysis are  
7 described. Numerical results are shown in section 3. Finally, concluding remarks are described  
8 in section 4.

9

## 10 **2. Theory**

### 11 ***2.1. Derivation of Transport Consistent Diffusion Coefficient***

12 The derivation of TCD coefficient is explained in this section. Firstly, the even-parity  
13 transport equation is derived followed by the explanation on the analytic solutions of even-  
14 parity and odd-parity angular fluxes. Secondly, the spatially averaged even-parity angular flux  
15 inside a mesh is obtained using the analytic solution of even-parity angular flux. Then the  
16 spatially averaged scalar flux inside a mesh is obtained by solid angle integration of the average  
17 even-parity angular flux. Thirdly, the neutron net current at mesh interface is derived by the  
18 solid angle integration of the odd-parity angular flux at the interface. Finally, the TCD  
19 coefficient is derived using Fick's law.

20 The transport equation for one-group, one-dimensional, homogeneous geometry with an  
21 isotropic source is written as:

$$\mu \frac{d}{dx} \psi(x, \mu) + \Sigma_t \psi(x, \mu) = \frac{1}{2} q, \quad (1)$$

22 where

23  $\mu$ : direction cosine,

24  $x$ : position,

- 1  $\Sigma_t$ : macroscopic total cross section,  
 2  $\psi(x, \mu)$ : angular flux for direction  $\mu$  and position  $x$ ,  
 3  $q$ : fixed source.

4 The transport equation for the opposite direction is given by:

$$-\mu \frac{d\psi}{dx} + \Sigma_t \psi(x, -\mu) = \frac{1}{2} q. \quad (2)$$

5 By adding and subtracting Equations (1) and (2), the following equations are obtained:

$$\mu \frac{d\psi^-}{dx} + \Sigma_t \psi^+(x, \mu) = \frac{1}{2} q, \quad (3)$$

$$\mu \frac{d\psi^+}{dx} + \Sigma_t \psi^-(x, \mu) = 0, \quad (4)$$

6 where  $\psi^+$  and  $\psi^-$  are the even- and odd-parity angular fluxes defined as:

$$\psi^+(x, \mu) \equiv \frac{\psi(x, \mu) + \psi(x, -\mu)}{2}, \quad (5)$$

$$\psi^-(x, \mu) \equiv \frac{\psi(x, \mu) - \psi(x, -\mu)}{2}. \quad (6)$$

7 By eliminating  $\psi^-$  using Equations (3) and (4), the even-parity transport equation is obtained:

$$-\mu^2 \frac{d}{dx} \frac{1}{\Sigma_t} \frac{d\psi^+}{dx} + \Sigma_t \psi^+(x, \mu) = \frac{1}{2} q. \quad (7)$$

8 Now let us consider a two-node problem shown in **Figure 1**, which is usually used to derive  
 9 the coupling coefficient of CMFD acceleration in the advanced nodal method [1]. Here,  $q_l$  and  
 10  $q_r$  are spatially uniform isotropic neutron sources,  $\psi_l$  and  $\psi_r$  are angular fluxes,  $\phi_l$  and  
 11  $\phi_r$  are scalar fluxes, respectively. Sizes for the left and the right meshes are  $h$  and the origin is  
 12 set at the mesh boundary between the left and right meshes. Spatially uniform total cross section  
 13  $\Sigma_t$  is considered. Reflective boundary condition is applied both for the left and right boundaries.

14 **(Figure 1)**

1 Equation (7) can be analytically solved using the following boundary conditions:

$$\begin{aligned}
 \psi_l^-(-h, \mu) &= 0, \\
 \psi_r^-(+h, \mu) &= 0, \\
 \psi_l^+(0, \mu) &= \psi_r^+(0, \mu), \\
 \psi_l^-(0, \mu) &= \psi_r^-(0, \mu),
 \end{aligned} \tag{8}$$

2 where  $h$  is the mesh width as shown in Figure 1. The first two are the reflective boundary  
 3 condition. The third and fourth ones correspond to the continuity condition at material interface.

4 The analytic solutions of even-parity angular fluxes are given by:

$$\psi_l^+(x, \mu) = \frac{2q_l - (q_l - q_r) \frac{\cosh\left(\frac{\Sigma_t(h+x)}{\mu}\right)}{\cosh\left(\frac{\Sigma_t h}{\mu}\right)}}{4\Sigma_t}, \tag{9}$$

$$\psi_r^+(x, \mu) = \frac{2q_r + (q_l - q_r) \frac{\cosh\left(\frac{\Sigma_t(h-x)}{\mu}\right)}{\cosh\left(\frac{\Sigma_t h}{\mu}\right)}}{4\Sigma_t}, \tag{10}$$

5 where  $q_l$  and  $q_r$  are fixed sources as shown in Figure 1.

6 Using Equations (9) and (10), the odd parity angular flux at the mesh interface  $\psi^-(0, \mu)$ ,  
 7 the spatially averaged even parity angular fluxes  $\bar{\psi}_l^+(\mu)$  and  $\bar{\psi}_r^+(\mu)$  are given by:

$$\psi_l^-(0, \mu) = \psi_r^-(0, \mu) = \frac{(q_l - q_r) \tanh\left(\frac{\Sigma_t h}{\mu}\right)}{4\Sigma_t}, \tag{11}$$

$$\bar{\psi}_l^+(\mu) = \left( \int_{-h}^0 \psi_l^+(x, \mu) dx \right) / h = \frac{2h\Sigma_t q_l - (q_l - q_r) \mu \tanh\left(\frac{\Sigma_t h}{\mu}\right)}{4h\Sigma_t^2}, \tag{12}$$

$$\bar{\psi}_r^+(\mu) = \left( \int_0^{+h} \psi_r^+(x, \mu) dx \right) / h = \frac{2h\Sigma_t q_r + (q_l - q_r) \mu \tanh\left(\frac{\Sigma_t h}{\mu}\right)}{4h\Sigma_t^2}. \tag{13}$$

8 Using Equations (11), (12), and (13), the net neutron current  $J$  at the mesh interface, the  
 9 average scalar fluxes for the left and the right meshes  $\bar{\phi}_l, \bar{\phi}_r$  are given by:

$$J = \int_{-1}^{+1} \frac{(q_l - q_r)\mu \tanh\left(\frac{\Sigma_t h}{\mu}\right)}{4\Sigma_t} d\mu, \quad (14)$$

$$\bar{\phi}_l = \int_{-1}^{+1} \frac{2h\Sigma_t q_l - (q_l - q_r)\mu \tanh\left(\frac{\Sigma_t h}{\mu}\right)}{4h\Sigma_t^2} d\mu, \quad (15)$$

$$\bar{\phi}_r = \int_{-1}^{+1} \frac{2h\Sigma_t q_r + (q_l - q_r)\mu \tanh\left(\frac{\Sigma_t h}{\mu}\right)}{4h\Sigma_t^2} d\mu. \quad (16)$$

1 Forcing the Fick's law, the following relation is obtained:

$$J = -D^{TCD} \frac{(\bar{\phi}_r - \bar{\phi}_l)}{h}, \quad (17)$$

2 where  $D^{TCD}$  is the transport consistent diffusion (TCD) coefficient.

3 By substituting Equations (14), (15), and (16) into Equation (17),  $D^{TCD}$  can be expressed  
4 as:

$$D^{TCD} = -\frac{Jh}{\bar{\phi}_r - \bar{\phi}_l} = \frac{1}{\Sigma_t} \frac{\tau^2 \int_{-1}^{+1} \mu \tanh\left(\frac{\tau}{\mu}\right) d\mu}{4\tau - 2 \int_{-1}^{+1} \mu \tanh\left(\frac{\tau}{\mu}\right) d\mu}, \quad (18)$$

5 where  $\tau = \Sigma_t h$  is the optical length of a mesh. It should be noted that  $D^{TCD}$  depends on  $\Sigma_t$   
6 and  $\tau$ , and but it does not depend on  $q_l$  and  $q_r$ .

7

## 8 **2.2. Convergence Analysis**

9 Convergence analysis of the CMFD acceleration is carried out using the linearized  
10 Fourier analysis. The analysis procedure has been published in many previous works [14]-[16]  
11 but somewhat complicated. Therefore, the detailed description of the linearized Fourier analysis  
12 is provided as the supplemental material of this paper. In the following, the fundamental  
13 equations used for the linearized Fourier analysis are described in order to clarify the condition  
14 of convergence analysis.

15 The neutron transport equation in one-dimensional slab geometry assuming the step  
16 characteristics is written as:

$$\mu_n \frac{\psi_{n,k+\frac{1}{2}}^{l+\frac{1}{2}} - \psi_{n,k-\frac{1}{2}}^{l+\frac{1}{2}}}{h} + \Sigma_t \left( f_n \psi_{n,k+\frac{1}{2}}^{l+\frac{1}{2}} + (1-f_n) \psi_{n,k-\frac{1}{2}}^{l+\frac{1}{2}} \right) = \Sigma_s \phi_k^l + q, \quad (19)$$

$$f_n = -\frac{\mu_n}{h\Sigma_t} + \frac{1}{1 - e^{-\frac{h\Sigma_t}{\mu_n}}}, \quad (20)$$

$$1 - f_n = \frac{\mu_n}{h\Sigma_t} - \frac{e^{-\frac{h\Sigma_t}{\mu_n}}}{1 - e^{-\frac{h\Sigma_t}{\mu_n}}},$$

$$\phi_k^{l+\frac{1}{2}} = \frac{1}{2} \sum_n w_n \left( f_n \psi_{n,k+\frac{1}{2}}^{l+\frac{1}{2}} + (1-f_n) \psi_{n,k-\frac{1}{2}}^{l+\frac{1}{2}} \right), \quad (21)$$

- 1 where
- 2  $\mu_n$ : direction cosine for direction  $n$ ,
- 3  $\psi$ : angular flux,
- 4  $\phi$ : scalar flux,
- 5  $h$ : mesh width,
- 6  $\Sigma_t$ : macroscopic total cross section,
- 7  $\Sigma_s$ : macroscopic scattering cross section,
- 8  $q$ : neutron source,
- 9  $f_n$ : weighting factor to calculate average angular flux,
- 10  $w$ : quadrature weight,  $\sum_n w_n = 2$ ,
- 11  $l$ : index of iteration,
- 12  $k$ : index of mesh,  $k + \frac{1}{2}$  indicates mesh interface between  $k + 1$  and  $k$ ,
- 13  $n$ : index of direction.

- 14 In the CMFD acceleration, the following difference equation is used to represent the
- 15 neutron net current.

$$J_{i+\frac{1}{2}}^{l+1} = -D^{FD}(\phi_{i+1}^{l+1} - \phi_i^{l+1}) + D_{i+\frac{1}{2}}^{cor,l+\frac{1}{2}}(\phi_{i+1}^{l+1} + \phi_i^{l+1}), \quad (22)$$

$$J_{i-\frac{1}{2}}^{l+1} = -D^{FD}(\phi_i^{l+1} - \phi_{i-1}^{l+1}) + D_{i-\frac{1}{2}}^{cor,l+\frac{1}{2}}(\phi_i^{l+1} + \phi_{i-1}^{l+1}),$$

1 where

$$D^{FD} = \frac{D}{ph}, \quad (23)$$

$$J_{i+\frac{1}{2}}^{l+\frac{1}{2}} = \frac{1}{2} \sum_n w_n \mu_n \psi_{n,i+\frac{1}{2}}^{l+\frac{1}{2}}, \quad (24)$$

$$J_{i-\frac{1}{2}}^{l+\frac{1}{2}} = \frac{1}{2} \sum_n w_n \mu_n \psi_{n,i-\frac{1}{2}}^{l+\frac{1}{2}},$$

$$D_{i+\frac{1}{2}}^{cor,l+\frac{1}{2}} = \frac{J_{i+\frac{1}{2}}^{l+\frac{1}{2}} + D^{FD}(\phi_{i+1}^{l+\frac{1}{2}} - \phi_i^{l+\frac{1}{2}})}{\phi_{i+1}^{l+\frac{1}{2}} + \phi_i^{l+\frac{1}{2}}}, \quad (25)$$

$$D_{i-\frac{1}{2}}^{cor,l+\frac{1}{2}} = \frac{J_{i-\frac{1}{2}}^{l+\frac{1}{2}} + D^{FD}(\phi_i^{l+\frac{1}{2}} - \phi_{i-1}^{l+\frac{1}{2}})}{\phi_i^{l+\frac{1}{2}} + \phi_{i-1}^{l+\frac{1}{2}}},$$

$$J_{i+\frac{1}{2}}^{l+\frac{1}{2}} = \frac{1}{2} \sum_n w_n \mu_n \psi_{n,i+\frac{1}{2}}^{l+\frac{1}{2}}, \quad (26)$$

$$J_{i-\frac{1}{2}}^{l+\frac{1}{2}} = \frac{1}{2} \sum_n w_n \mu_n \psi_{n,i-\frac{1}{2}}^{l+\frac{1}{2}},$$

2 and

3  $D$ : diffusion coefficient,  $i$ : index of coarse mesh,  $i + \frac{1}{2}$  indicates mesh interface between  $i +$

4 1 and  $i$ ,  $p$ : number of fine meshes in a coarse mesh.

5 Using Equation (22), the CMFD equation is written as:



$$\begin{aligned}
& -D_{i+\frac{1}{2}}(\phi_{i+1}^{l+1} - \phi_i^{l+1}) + D_{i+\frac{1}{2}}^{cor,l+\frac{1}{2}}(\phi_{i+1}^{l+1} + \phi_i^{l+1}) + D_{i-\frac{1}{2}}(\phi_i^{l+1} - \phi_{i-1}^{l+1}) \\
& - D_{i-\frac{1}{2}}^{cor,l+\frac{1}{2}}(\phi_i^{l+1} + \phi_{i-1}^{l+1}) + ph\Sigma_a\phi_i^{l+1} = phq,
\end{aligned} \tag{27}$$

1 where  $\Sigma_a = \Sigma_t - \Sigma_s$ .

2 Once the CMFD solution is obtained, the scalar flux is normalized as:

$$\phi_k^{l+1} = \phi_k^{l+\frac{1}{2}} \frac{\phi_i^{l+1}}{\phi_i^{l+\frac{1}{2}}}. \tag{28}$$

3 Equations (19), (25)-(28) consist a set for CMFD acceleration. These equations are used for the  
4 convergence analysis using the linearized Fourier analysis.

5

### 6 **3. Numerical Results and Discussions**

#### 7 **3.1. Comparison of Diffusion Coefficients**

8 The transport consistent diffusion (TCD) coefficient derived in section 2.1 is compared  
9 with the conventional diffusion coefficient (ConvD), the effective diffusion coefficient (EffD),  
10 and the artificial grid diffusion coefficient (AGD). The definitions of ConvD, EffD, and AGD  
11 are as follows:

$$D^{ConvD} = \frac{1}{3\Sigma_t}, \tag{29}$$

$$D^{EffD} = \frac{1}{3\Sigma_t} + \frac{\tau}{4\Sigma_t} \int_{-1}^{+1} \left( \frac{1 + \exp\left(-\frac{\tau}{\mu}\right)}{1 - \exp\left(-\frac{\tau}{\mu}\right)} - \frac{2\mu}{\tau} \right) \mu d\mu, \tag{30}$$

$$D^{AGD} = \frac{1}{3\Sigma_t} + \frac{\tau}{4\Sigma_t}. \tag{31}$$

12 Comparison of the diffusion coefficients is shown in **Figure 2**. Note that dimensionless  
13 parameter,  $D\Sigma_t$ , is shown. Behavior of  $D^{TCD}$  is similar to those of  $D^{EffD}$  and  $D^{AGD}$  while  
14 that of  $D^{ConvD}$  is different.

1 (Figure 2)

2 When the optical thickness of a mesh  $\tau$  is large,  $D^{TCD}$  and  $D^{EffD}$  can be  
3 approximated by:

$$D^{TCD} \approx \frac{1}{\Sigma_t} \frac{\tau^2}{4\tau - 2} \approx \frac{1}{4\Sigma_t} \left( \tau + \frac{1}{2} \right), \quad (32)$$

$$D^{EffD} \approx \frac{1}{3\Sigma_t} + \frac{1}{4\Sigma_t} \left( \tau - \frac{4}{3} \right). \quad (33)$$

4 The approximated  $D^{TCD}$  and  $D^{EffD}$  are shown in **Figure 3**.

5 (Figure 3)

6 By comparing Equations (31), (32), and (33), the dependence of these diffusion  
7 coefficients on the optical mesh size  $\tau$  is characterized by  $\frac{\tau}{4\Sigma_t}$ . Reference [13] revealed that  
8 the stabilization effect of  $D^{EffD}$  and  $D^{AGD}$  are similar. This suggests that utilization of  $D^{TCD}$   
9 will also contribute to improve stability of the CMFD/GCMR acceleration methods.

10 **Figure 4** indicates the relation between optical length and  $D/h$ . It is interesting that  
11  $D^{TCD}/h$  converges to a finite value ( $\sim 0.586$ ) when  $\tau$  approaches 0. It means that  $D^{TCD}$  gives  
12 a finite diffusion coefficient for a void region with a finite mesh size, which would have a  
13 positive impact on convergence of the CMFD/GCMR acceleration.

14 (Figure 4)

### 16 3.2. Convergence Estimation using the Linearized Fourier Analysis

17 Three major parameters affecting the convergence of the CMFD acceleration are  
18 considered in the linearized Fourier analysis as follows:

- 19 •Scattering ratio ( $\Sigma_s/\Sigma_t$ ): 0.99
- 20 •Number of fine meshes in a coarse mesh: 1, 4
- 21 •Optical thickness of a coarse mesh:  $10^{-2}$ – $10^2$

22 The results of linearized Fourier analysis for four different diffusion coefficients are

1 shown in **Figures 5** and **6**. The results indicate that  $D^{EffD}$ ,  $D^{AGD}$ , and  $D^{TCD}$  show similar  
 2 convergent behavior for optically thick meshes, which increases convergence stability. Contrary,  
 3 the spectral radius of  $D^{TCD}$  becomes large for an optically thin mesh. The numerical result  
 4 show that  $D^{TCD}/h$  approaches approximately 0.6 for an optically thin mesh. The previous  
 5 study [4] revealed that the CMFD acceleration method is consistent with the coarse mesh  
 6 rebalance (CMR) when  $D/h = 1/2$ . Therefore, the performance of  $D^{TCD}$  would be similar to  
 7 that of CMR for optically thin meshes. Performance of these diffusion coefficient in actual  
 8 heterogeneous geometry will be confirmed in section 3.2.

9 **(Figure 5)**

10 **(Figure 6)**

### 11 **3.3. Convergence Estimation in C5G7 3D benchmark problem**

12 The TCD is derived assuming a very simplified condition (one-group, one-dimensional  
 13 slab geometry with a uniform fixed source in each region) and the linearized Fourier analysis  
 14 also assumes a simplified condition. Therefore, its performance evaluation in more realistic  
 15 conditions is desirable. In this section, the impact of diffusion coefficient on the convergence  
 16 of the CMFD acceleration is verified through the C5G7 3D benchmark problem [17]. In the  
 17 original C5G7 benchmark problem, the non-voided condition is specified but the voided  
 18 condition is also considered in this study. The GENESIS code, which is a three-dimensional  
 19 transport code based on the Legendre polynomial Expansion of Angular Flux (LEAF) method,  
 20 is used [18]. The calculation conditions are as summarized as follows:

- 22 •Number of azimuthal angles: 8 for  $2\pi$
- 23 •Number of polar angles(Gauss-Legendre): 4 for  $\pi$
- 24 •Ray trace width: 0.2 cm
- 25 •Axial mesh size: 3.0 cm
- 26 •Radial mesh division: **Figure 7**

- 1 •Number of inner iterations: 1 or 2
- 2 •Convergence criterion for k-effective:  $5 \times 10^{-6}$
- 3 •Convergence criterion scalar flux:  $1 \times 10^{-5}$
- 4 •Mesh size for CMFD: 1 cell and 3.0 cm for radial and axial directions,
- 5 respectively

6 **(Figure 7)**

7 The above discretization parameters are too coarse to obtain the converged results [18]  
 8 but they are appropriate in the present study since the evaluation of convergence behavior of  
 9 the CMFD acceleration is the major purpose in this paper and the convergence behavior of the  
 10 CMFD acceleration is not very sensitive to the discretization parameters. It should be also noted  
 11 the damping factor [10][13] is not used to stabilize the CMFD acceleration. The specification  
 12 of the voided condition is taken from Ref.[18].

13 Calculation results are shown in **Figures 8** and **9**. Note that each CMFD calculation has  
 14 been fully converged in each acceleration. Performances of  $D^{EffD}$ ,  $D^{AGD}$ , and  $D^{TCD}$  are  
 15 similar in the non-voided case, while  $D^{TCD}$  shows better performance in the voided case. This  
 16 result seems to be somewhat inconsistent with that of the linearized Fourier analysis since  
 17 convergence performance of  $D^{TCD}$  is worse than  $D^{EffD}$  and  $D^{AGD}$  for an optically thin  
 18 mesh. A possible reason of the better convergence of  $D^{TCD}$  would be the value of diffusion  
 19 coefficients. The value of  $D^{EffD}$ ,  $D^{AGD}$ , and  $D^{ConvD}$  could become large for voided region,  
 20 which has a negative impact on the convergence of a diffusion calculation, while that of  $D^{TCD}$   
 21 is finite. This might be a cause of the difference of convergence behavior observed in the voided  
 22 case. However, further study on the convergence property of CMFD acceleration in realistic  
 23 heterogeneous geometry will be desirable to clarify and to understand this issue. For example,  
 24 linearized Fourier analysis considering different total cross sections and the periodic boundary  
 25 condition would be an approach to address this question. Such a study, unfortunately, requires  
 26 considerable new development works thus is considered as a future task.

1 (Figure 8)

2 (Figure 9)

3  
4 **4. Conclusion**

5 The transport consistent diffusion (TCD) coefficient is derived using the even-parity  
6 transport equation and the two-node problem in one-dimensional geometry. TCD depends on  
7 the optical mesh size and shows similar behavior with the effective diffusion (EffD) and the  
8 artificial grid diffusion (AGD) coefficients for an optically thick mesh.

9 Convergence performances of TCD, AGD, EffD, and conventional diffusion coefficient  
10 (ConvD) are compared through the linearized Fourier analysis and numerical calculations in  
11 the C5G7 3D benchmark problem. The linearized Fourier analysis indicates that TCD, AGD,  
12 and EffD show similar theoretical convergence behavior for an optically thick mesh. In the  
13 C5G7 3D benchmark problem, TCD, AGD, and EffD show better performance than ConvD in  
14 the non-voided and voided conditions. In the voided condition, TCD is superior to AGD and  
15 EffD. This reason would be the limited value of TCD, which does not become very large for a  
16 voided region. However, further investigation on better performance of TCD in highly voided  
17 condition would be desirable, *e.g.*, linearized Fourier analysis considering different total cross  
18 sections and the periodic boundary condition.

19 The above results suggest that the TCD will be a candidate for the CMFD acceleration  
20 which can be robustly used not only for conventional calculation conditions but also for highly  
21 voided conditions.  
22  
23

## 1 **References**

- 2 [1] Smith K. Nodal method storage reduction by non-linear iteration. *Trans. Am. Nucl. Soc.*  
3 1983; 44: 265–266.
- 4 [2] Smith K, Rhodes JD. Full-core, 2-D, LWR core calculations with CASMO-4E. *Proc.*  
5 *PHYSOR2002*; 2002 Oct 7–10; Seoul (South Korea). [CD-ROM].
- 6 [3] Joo HG, Cho JY, Kim KS, Lee CC, Zee SQ. Methods and performance of a three-  
7 dimensional whole-core transport code DeCART. *Proc. PHYSOR2004*; 2004 Apr 25–29;  
8 Chicago Illinois (US). [CD-ROM].
- 9 [4] Yamamoto A. Generalized coarse mesh rebalance method for acceleration of neutron  
10 transport calculations. *Nucl. Sci. Eng.* 2005; 151: 274–282.
- 11 [5] Yamamoto A, Endo T, Tabuchi M, Sugimura N, Ushio T, Mori M, Tatsumi M, Ohoka Y.  
12 AEGIS: An Advanced Lattice Physics Code for Light Water Reactor Analyses. *Nucl. Eng.*  
13 *Technol.* 2010; 42: 500–519.
- 14 [6] Jung YS, Shim CB, Lim CH, Joo HG. Practical numerical reactor employing direct whole  
15 core neutron transport and subchannel thermal/hydraulic solvers. *Ann. Nucl. Energy.* 2013;  
16 62:357–374
- 17 [7] Boyd W, Shaner W, Li L, Forget B, Smith K, The OpenMOC Method of Characteristics  
18 Neutral Particle Transport Code. *Ann. Nucl. Energy.* 2014; 68: 43–52.
- 19 [8] Zhu A, Transient Methods for Pin-Resolved Whole Core Transport using the 2D-1D  
20 Methodology in MPACT. *Proc. M&C2015*; 2015 Apr 19–23; Nashville Tennessee (US).  
21 [USB-DRIVE].
- 22 [9] Chen J, Liu Z, Zhao C, He Q, Zu T, Cao, L, Wu H., A new high-fidelity neutronics code  
23 NECP-X. *Ann. Nucl. Energy* 2018; 116: 417–428.
- 24 [10] Jarrett M, Kochunas B, Zhu A, Downar T. Analysis of stabilization techniques for CMFD  
25 acceleration of neutron transport problems. *Nucl. Sci. Eng.* 2016; 184: 208–227.

- 1 [11] Larsen E. Infinite medium solutions to the transport equation, Sn discretization schemes,  
2 and the diffusion approximation. Proc. of the Joint International Topical Meeting on  
3 Mathematics and Computation and Supercomputing in Nuclear Applications; 2001 Sep 9–  
4 13; Salt Lake City, UT, (USA). [CD-ROM].
- 5 [12] Cho NZ, Lee GS, Park CJ. Partial current-based CMFD acceleration of the 2D/1D fusion  
6 method for 3D whole-core transport calculations. Trans. Am. Nucl. Soc. 2003; 88: 594–596.
- 7 [13] Yamamoto A, Giho A, Endo T. Recent Developments in the GENESIS code based on the  
8 Legendre polynomial expansion of angular flux method. Nucl. Eng. Technol. 2017;  
9 49:1143–1156.
- 10 [14] Cefus GR, Larsen EW. Stability analysis of the coarse-mesh rebalance. Nucl. Sci. Eng.  
11 1990; 105: 31–39.
- 12 [15] Hong SG, Kim KS, Song JS. Fourier convergence analysis of the rebalance methods for  
13 discrete ordinates transport equations in eigenvalue problems. Nucl. Sci. Eng. 2010; 164:  
14 33–52.
- 15 [16] Kim HT, Kim Y. Convergence studies on nonlinear coarse-mesh finite difference  
16 accelerations for neutron transport analysis. Nucl. Sci. Eng. 2018; 191: 136–149.
- 17 [17] Benchmark on Deterministic Transport calculations without spatial homogenisation—  
18 MOX fuel assembly 3-d extension case. NEA/NSC/DOC(2005)16. 2005. Organisation for  
19 Economic Co-operation and Development/Nuclear Energy Agency.
- 20 [18] Yamamoto A, Giho A, Kato Y, Endo T. GENESIS - a three-dimensional heterogeneous  
21 transport solver based on the Legendre polynomial expansion of angular flux method. Nucl.  
22 Sci. Eng. 2017; 186: 1–22.
- 23

## Figure captions

Figure 1. Two-node problem

Figure 2. Comparison of diffusion coefficients ( $\tau = \Sigma_t h$  versus  $D\Sigma_t$ )

Figure 3. Approximated  $D^{TCD}$  and  $D^{EffD}$  ( $\tau = \Sigma_t h$  versus  $D\Sigma_t$ )

Figure 4. Comparison of diffusion coefficients ( $\tau = \Sigma_t h$  versus  $D/h$ )

Figure 5. Comparison of spectral radius ( $c=0.99, p=1$ )

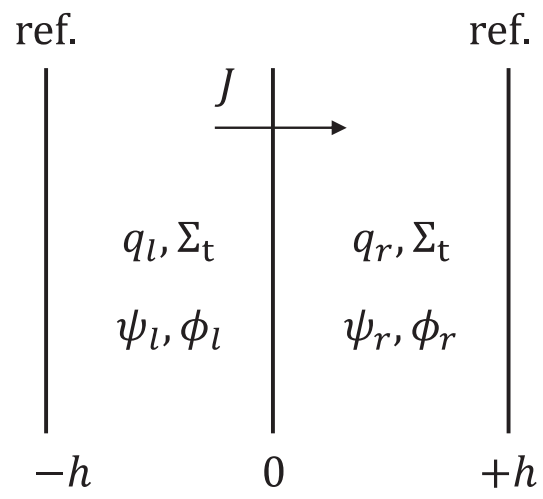
Figure 6. Comparison of spectral radius ( $c=0.99, p=4$ )

Figure 7. Mesh division used in the C5G7 3D benchmark problem

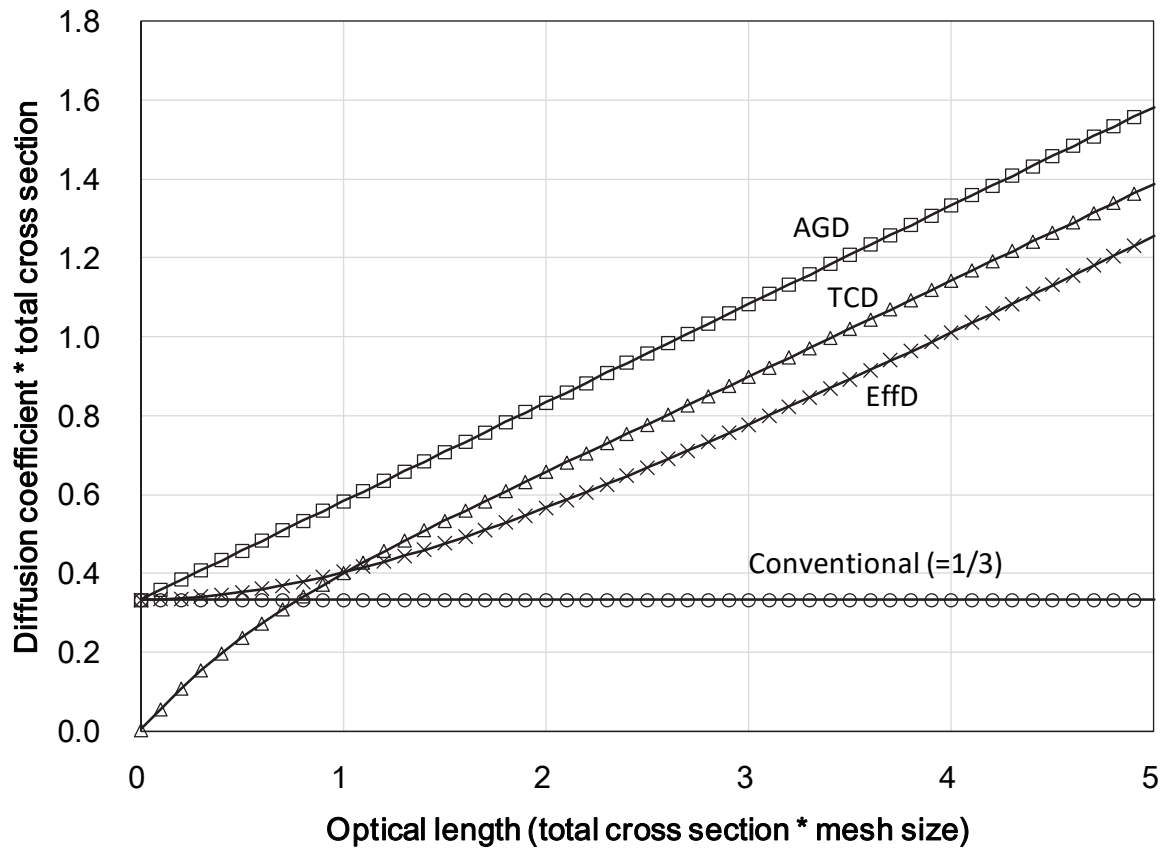
Figure 8. Comparison of number of outer iterations of the C5G7 benchmark problem (non-voided case)

Figure 9. Comparison of number of outer iterations of the C5G7 benchmark problem (voided case)

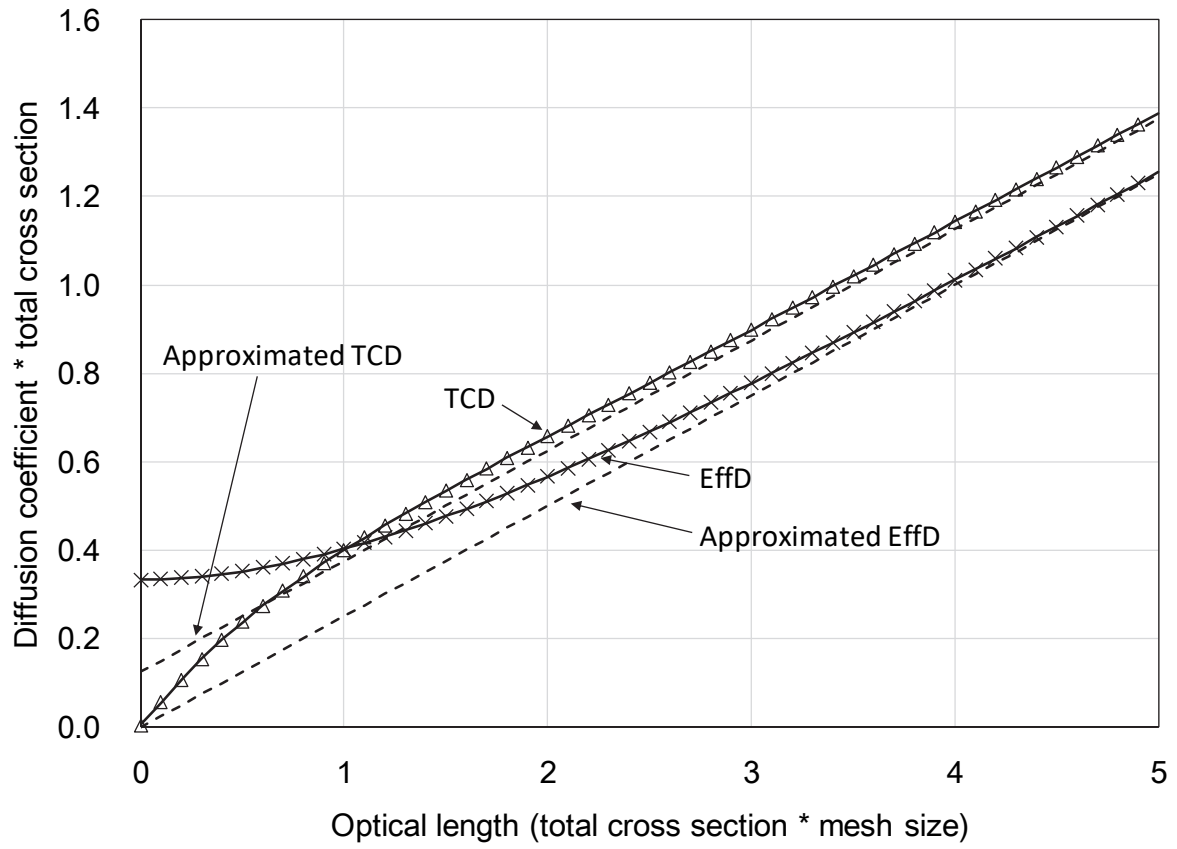




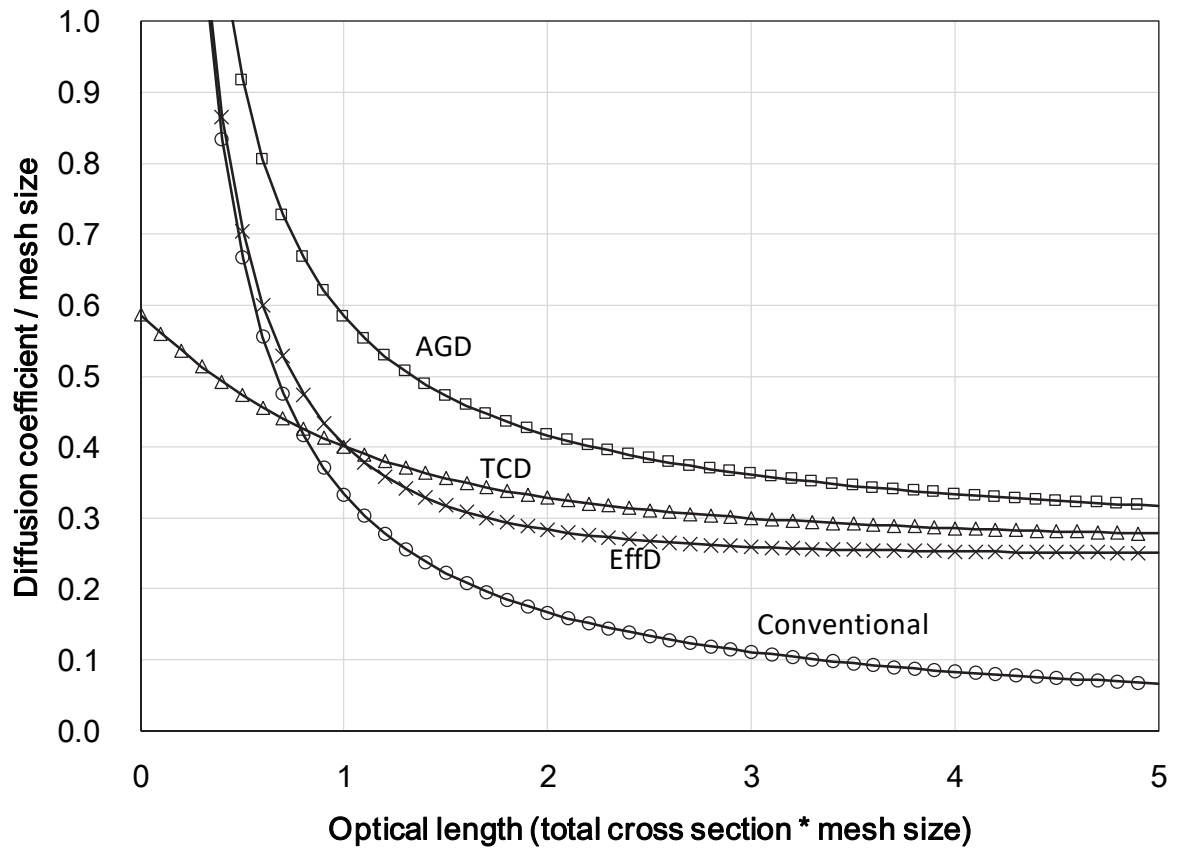
**Figure 1.** Two-node problem



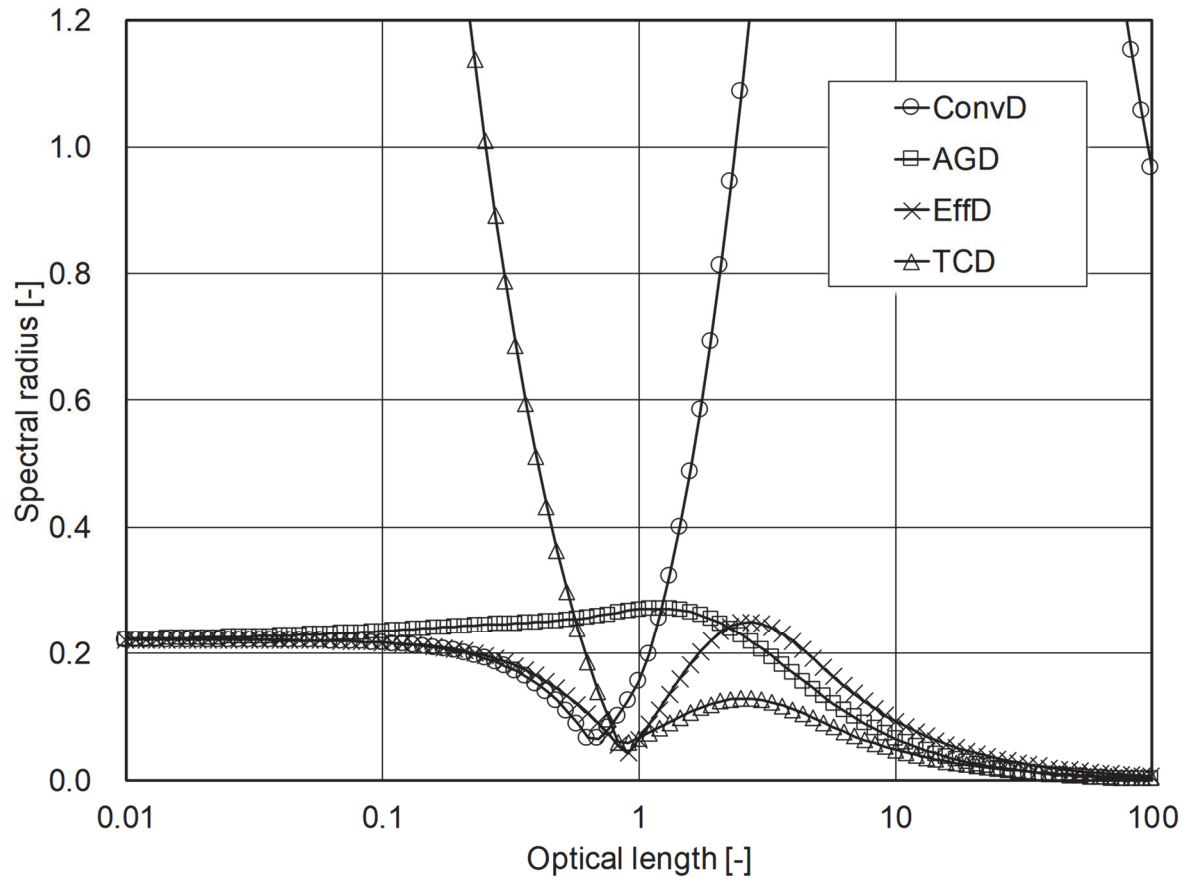
**Figure 2.** Comparison of diffusion coefficients ( $\tau = \Sigma_t h$  versus  $D\Sigma_t$ )



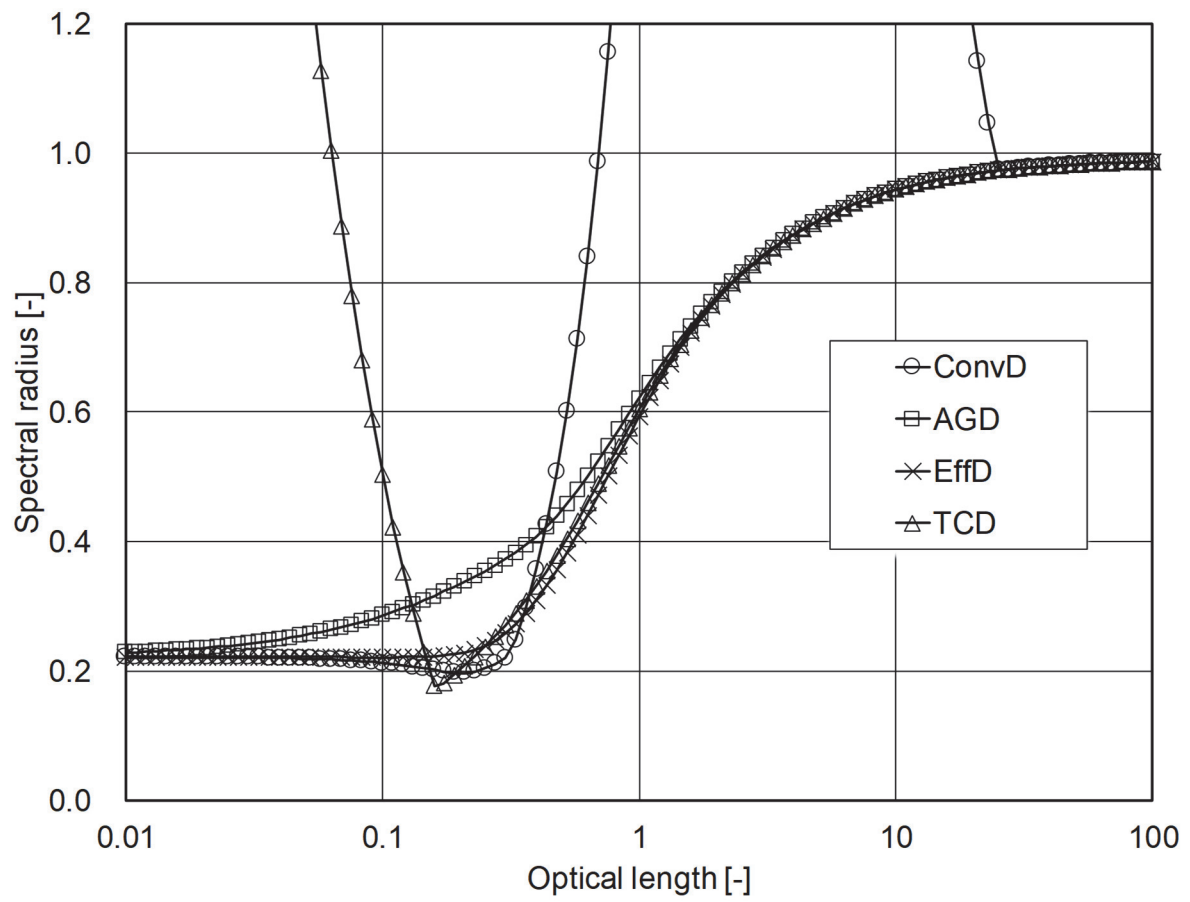
**Figure 3.** Approximated  $D^{TCD}$  and  $D^{EffD}$  ( $\tau = \Sigma_t h$  versus  $D\Sigma_t$ )



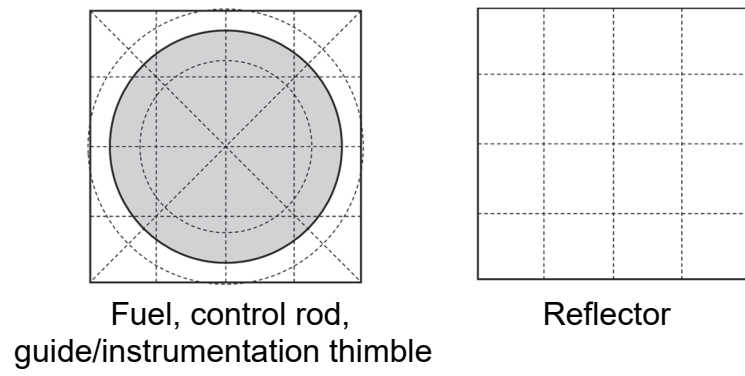
**Figure 4.** Comparison of diffusion coefficients ( $\tau = \Sigma_t h$  versus  $D/h$ )



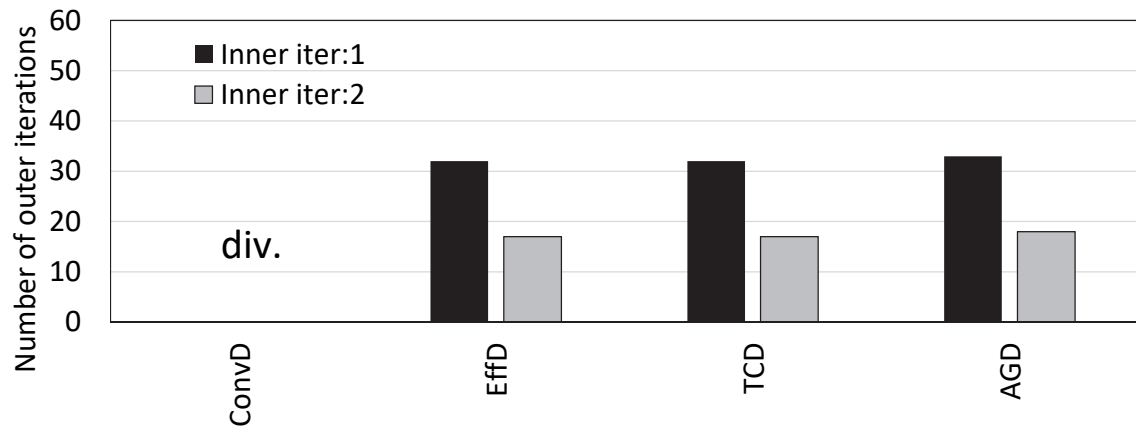
**Figure 5.** Comparison of spectral radius ( $c=0.99, p=1$ )



**Figure 6.** Comparison of spectral radius ( $c=0.99, p=4$ )

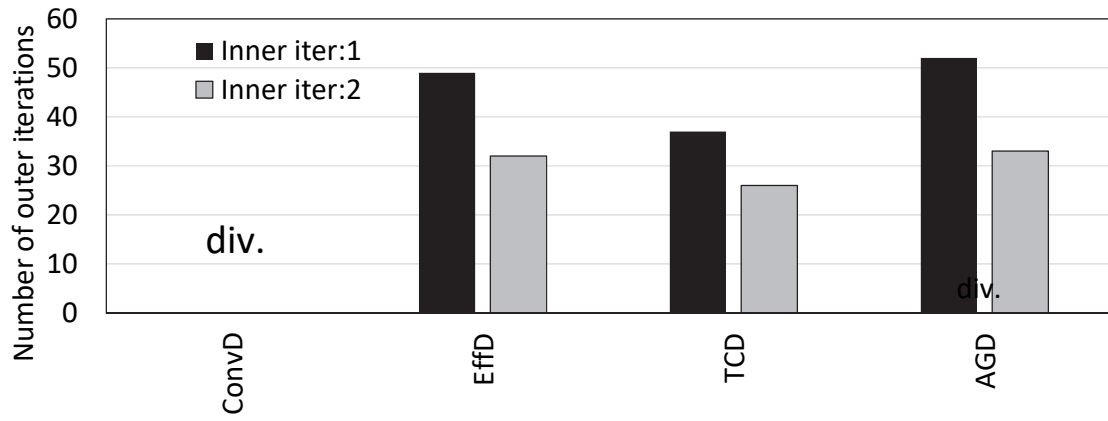


**Figure 7.** Mesh division used in the C5G7 3D benchmark problem



**Figure 8.** Comparison of number of outer iterations of the C5G7 benchmark problem (non-voided case)





**Figure 9.** Comparison of number of outer iterations of the C5G7 benchmark problem (voided case)

**Supplemental material of “Transport consistent diffusion coefficient for CMFD acceleration and comparison of convergence properties” by A. Yamamoto et al.**

Detail derivation for the linearized Fourier analysis is described in this supplemental material. Though part of the derivation is described in the paper, complete derivation is provided for completeness of this document. The following derivation is based on Refs.[3], [4], [8], and [10].

**1. Fundamental formulations**

The neutron transport equation in one-dimensional slab geometry using the step characteristics approximation is written as:

$$\mu_n \frac{\psi_{n,k+\frac{1}{2}}^{l+\frac{1}{2}} - \psi_{n,k-\frac{1}{2}}^{l+\frac{1}{2}}}{h} + \Sigma_t \left( f_n \psi_{n,k+\frac{1}{2}}^{l+\frac{1}{2}} + (1 - f_n) \psi_{n,k-\frac{1}{2}}^{l+\frac{1}{2}} \right) = \Sigma_s \phi_k^l + q, \quad (1)$$

$$f_n = -\frac{\mu_n}{h\Sigma_t} + \frac{1}{1 - e^{-\frac{h\Sigma_t}{\mu_n}}}, \quad (2)$$

$$1 - f_n = \frac{\mu_n}{h\Sigma_t} - \frac{e^{-\frac{h\Sigma_t}{\mu_n}}}{1 - e^{-\frac{h\Sigma_t}{\mu_n}}},$$

$$\phi_k^{l+\frac{1}{2}} = \frac{1}{2} \sum_n w_n \left( f_n \psi_{n,k+\frac{1}{2}}^{l+\frac{1}{2}} + (1 - f_n) \psi_{n,k-\frac{1}{2}}^{l+\frac{1}{2}} \right), \quad (3)$$

where

$\mu_n$ : direction cosine for direction  $n$ ,

$\psi$ : angular flux,

$\phi$ : scalar flux,

$h$ : mesh width,

$\Sigma_t$ : macroscopic total cross section,

$\Sigma_s$ : macroscopic scattering cross section,

$q$ : isotropic neutron source,

$f_n$ : weighting factor to calculate average angular flux for direction  $n$ ,

$w$ : quadrature weight,  $\sum_n w_n = 2$ ,

$l$ : index of iteration,

$k$ : index of mesh,  $k + \frac{1}{2}$  indicates mesh interface between  $k + 1$  and  $k$ ,

$n$ : index of direction.

In the CMFD acceleration, the following difference equation is used for the neutron net current.

$$\begin{aligned}
J_{i+\frac{1}{2}}^{l+1} &= -D^{FD}(\phi_{i+1}^{l+1} - \phi_i^{l+1}) + D_{i+\frac{1}{2}}^{cor,l+\frac{1}{2}}(\phi_{i+1}^{l+1} + \phi_i^{l+1}), \\
J_{i-\frac{1}{2}}^{l+1} &= -D^{FD}(\phi_i^{l+1} - \phi_{i-1}^{l+1}) + D_{i-\frac{1}{2}}^{cor,l+\frac{1}{2}}(\phi_i^{l+1} + \phi_{i-1}^{l+1}),
\end{aligned} \tag{4}$$

where,

$$D^{FD} = \frac{D}{ph}, \tag{5}$$

$$D_{i+\frac{1}{2}}^{cor,l+\frac{1}{2}} = \frac{J_{i+\frac{1}{2}}^{l+\frac{1}{2}} + D^{FD}(\phi_{i+1}^{l+\frac{1}{2}} - \phi_i^{l+\frac{1}{2}})}{\phi_{i+1}^{l+\frac{1}{2}} + \phi_i^{l+\frac{1}{2}}}, \tag{6}$$

$$D_{i-\frac{1}{2}}^{cor,l+\frac{1}{2}} = \frac{J_{i-\frac{1}{2}}^{l+\frac{1}{2}} + D^{FD}(\phi_i^{l+\frac{1}{2}} - \phi_{i-1}^{l+\frac{1}{2}})}{\phi_i^{l+\frac{1}{2}} + \phi_{i-1}^{l+\frac{1}{2}}},$$

$$J_{i+\frac{1}{2}}^{l+\frac{1}{2}} = \frac{1}{2} \sum_n w_n \mu_n \psi_{n,i+\frac{1}{2}}^{l+\frac{1}{2}}, \tag{7}$$

$$J_{i-\frac{1}{2}}^{l+\frac{1}{2}} = \frac{1}{2} \sum_n w_n \mu_n \psi_{n,i-\frac{1}{2}}^{l+\frac{1}{2}},$$

and

$D$ : diffusion coefficient,  $i$ : index of coarse mesh,  $i + \frac{1}{2}$  indicates coarse mesh interface between  $i + 1$  and  $i$ , and a coarse mesh include  $p$  fine meshes.

Using Eq.(4), the CMFD equation is written as:

$$\begin{aligned}
&-D^{FD}(\phi_{i+1}^{l+1} - \phi_i^{l+1}) + D_{i+\frac{1}{2}}^{cor,l+\frac{1}{2}}(\phi_{i+1}^{l+1} + \phi_i^{l+1}) + D^{FD}(\phi_i^{l+1} - \phi_{i-1}^{l+1}) \\
&- D_{i-\frac{1}{2}}^{cor,l+\frac{1}{2}}(\phi_i^{l+1} + \phi_{i-1}^{l+1}) + ph\Sigma_a\phi_i^{l+1} = phq,
\end{aligned} \tag{8}$$

where  $\Sigma_a = \Sigma_t - \Sigma_s$ .

Once the CMFD solution is obtained, the scalar flux is normalized as:

$$\phi_k^{l+1} = \phi_k^{l+\frac{1}{2}} \frac{\phi_i^{l+1}}{\phi_i^{l+\frac{1}{2}}}. \tag{9}$$

Equations (1), (6)-(9) consist a set for the CMFD acceleration.

## 2. Fourier analysis

### 2.1 Relation of angular flux errors in transport equation

The following expansions are used:

$$\begin{aligned}
\phi_i^l &= \frac{q}{\Sigma_a} (1 + \varepsilon \zeta_i^l), \\
\phi_i^{l+\frac{1}{2}} &= \frac{q}{\Sigma_a} \left( 1 + \varepsilon \zeta_i^{l+\frac{1}{2}} \right), \\
\phi_k^l &= \frac{q}{\Sigma_a} (1 + \varepsilon \zeta_k^l), \\
\phi_k^{l+\frac{1}{2}} &= \frac{q}{\Sigma_a} \left( 1 + \varepsilon \zeta_k^{l+\frac{1}{2}} \right), \\
\psi_{n,i+\frac{1}{2}}^{l+\frac{1}{2}} &= \frac{q}{\Sigma_a} \left( 1 + \varepsilon \xi_{n,i+\frac{1}{2}}^{l+\frac{1}{2}} \right), \\
\psi_{n,k+\frac{1}{2}}^{l+\frac{1}{2}} &= \frac{q}{\Sigma_a} \left( 1 + \varepsilon \xi_{n,k+\frac{1}{2}}^{l+\frac{1}{2}} \right).
\end{aligned} \tag{10}$$

Substitute Eq.(10) into Eq.(1) and divide both sides by  $\Sigma_t$ , we have:

$$\begin{aligned}
\mu_n \frac{1}{h \Sigma_t} & \left( \frac{q}{\Sigma_a} \left( 1 + \varepsilon \xi_{n,k+\frac{1}{2}}^{l+\frac{1}{2}} \right) - \frac{q}{\Sigma_a} \left( 1 + \varepsilon \xi_{n,k-\frac{1}{2}}^{l+\frac{1}{2}} \right) \right) \\
& + \left( f_n \frac{q}{\Sigma_a} \left( 1 + \varepsilon \xi_{n,k+\frac{1}{2}}^{l+\frac{1}{2}} \right) + (1 - f_n) \frac{q}{\Sigma_a} \left( 1 + \varepsilon \xi_{n,k-\frac{1}{2}}^{l+\frac{1}{2}} \right) \right) \\
& = \frac{\Sigma_s}{\Sigma_t} \frac{q}{\Sigma_a} (1 + \varepsilon \zeta_k^l) + \frac{q}{\Sigma_t}.
\end{aligned} \tag{11}$$

Equation (11) can be written as:

$$\begin{aligned}
\mu_n \frac{1}{h \Sigma_t} & \left( \frac{q}{\Sigma_a} \left( \varepsilon \xi_{n,k+\frac{1}{2}}^{l+\frac{1}{2}} - \varepsilon \xi_{n,k-\frac{1}{2}}^{l+\frac{1}{2}} \right) \right) + \left( \frac{q}{\Sigma_a} \left( f_n \varepsilon \xi_{n,k+\frac{1}{2}}^{l+\frac{1}{2}} + (1 - f_n) \varepsilon \xi_{n,k-\frac{1}{2}}^{l+\frac{1}{2}} \right) \right) \\
& = \frac{\Sigma_s}{\Sigma_t} \frac{q}{\Sigma_a} \varepsilon \zeta_k^l,
\end{aligned} \tag{12}$$

where the following relation is considered:

$$\frac{\Sigma_s}{\Sigma_t} \frac{q}{\Sigma_a} + \frac{q}{\Sigma_t} = \frac{\Sigma_s q + \Sigma_a q}{\Sigma_t \Sigma_a} = \frac{\Sigma_t q}{\Sigma_t \Sigma_a} = \frac{q}{\Sigma_a}. \tag{13}$$

Equation (12) can be further simplified as:

$$\mu_n \frac{1}{h \Sigma_t} \left( \xi_{n,k+\frac{1}{2}}^{l+\frac{1}{2}} - \xi_{n,k-\frac{1}{2}}^{l+\frac{1}{2}} \right) + \left( f_n \xi_{n,k+\frac{1}{2}}^{l+\frac{1}{2}} + (1 - f_n) \xi_{n,k-\frac{1}{2}}^{l+\frac{1}{2}} \right) = c \zeta_k^l, \tag{14}$$

where  $c = \frac{\Sigma_s}{\Sigma_t}$ .

Substituting Eq. (10) into Eq. (3), we have:

$$\zeta_k^{l+\frac{1}{2}} = \frac{1}{2} \sum_n w_n \left( f_n \xi_{n,k+\frac{1}{2}}^{l+\frac{1}{2}} + (1 - f_n) \xi_{n,k-\frac{1}{2}}^{l+\frac{1}{2}} \right). \quad (15)$$

Equations (14) and (15) represent errors during the transport iterations.

## 2.2 Relation of scalar flux errors in CMFD equation

Next, we will derive similar formulation for the CMFD equation. Multiplying both sides of Eq.(6) by  $(\phi_{i+1}^{l+1} + \phi_i^{l+1})$ , we have the following:

$$D_{i+\frac{1}{2}}^{cor,l+\frac{1}{2}}(\phi_{i+1}^{l+1} + \phi_i^{l+1}) = \left( J_{i+\frac{1}{2}}^{l+\frac{1}{2}} + D^{FD} \left( \phi_{i+1}^{l+\frac{1}{2}} - \phi_i^{l+\frac{1}{2}} \right) \right) \frac{\phi_{i+1}^{l+1} + \phi_i^{l+1}}{\phi_{i+1}^{l+\frac{1}{2}} + \phi_i^{l+\frac{1}{2}}}. \quad (16)$$

Inserting Eqs.(7) and (10) into Eq.(16), we have:

$$\begin{aligned}
& D_{i+\frac{1}{2}}^{cor,l+\frac{1}{2}}(\phi_{i+1}^{l+1} + \phi_i^{l+1}) \\
&= \left( \frac{1}{2} \sum_n w_n \mu_n \frac{q}{\Sigma_a} \left( 1 + \varepsilon \xi_{n,i+\frac{1}{2}}^{l+\frac{1}{2}} \right) \right. \\
&\quad + D^{FD} \left( \frac{q}{\Sigma_a} \left( 1 + \varepsilon \zeta_{i+1}^{l+\frac{1}{2}} \right) \right. \\
&\quad \left. \left. - \frac{q}{\Sigma_a} \left( 1 + \varepsilon \zeta_i^{l+\frac{1}{2}} \right) \right) \right) \frac{\frac{q}{\Sigma_a} (1 + \varepsilon \zeta_{i+1}^{l+1}) + \frac{q}{\Sigma_a} (1 + \varepsilon \zeta_i^{l+1})}{\frac{q}{\Sigma_a} (1 + \varepsilon \zeta_{i+1}^{l+\frac{1}{2}}) + \frac{q}{\Sigma_a} (1 + \varepsilon \zeta_i^{l+\frac{1}{2}})} \\
&= \left( \frac{1}{2} \sum_n w_n \mu_n \frac{q}{\Sigma_a} \left( 1 + \varepsilon \xi_{n,i+\frac{1}{2}}^{l+\frac{1}{2}} \right) \right. \\
&\quad \left. + D^{FD} \frac{q}{\Sigma_a} \left( \varepsilon \zeta_{i+1}^{l+\frac{1}{2}} - \varepsilon \zeta_i^{l+\frac{1}{2}} \right) \right) \left( \frac{1 + \varepsilon \zeta_{i+1}^{l+1} + 1 + \varepsilon \zeta_i^{l+1}}{1 + \varepsilon \zeta_{i+1}^{l+\frac{1}{2}} + 1 + \varepsilon \zeta_i^{l+\frac{1}{2}}} \right) \tag{17} \\
&= \left( \frac{1}{2} \sum_n w_n \mu_n \frac{q}{\Sigma_a} \left( 1 + \varepsilon \xi_{n,i+\frac{1}{2}}^{l+\frac{1}{2}} \right) + D^{FD} \frac{q}{\Sigma_a} \left( \varepsilon \zeta_{i+1}^{l+\frac{1}{2}} - \varepsilon \zeta_i^{l+\frac{1}{2}} \right) \right) \left( 1 \right. \\
&\quad \left. + \frac{\varepsilon}{2} \left( \zeta_{i+1}^{l+1} + \zeta_i^{l+1} - \zeta_{i+1}^{l+\frac{1}{2}} - \zeta_i^{l+\frac{1}{2}} \right) + O(\varepsilon^2) \right) \\
&= \frac{1}{2} \sum_n w_n \mu_n \frac{q}{\Sigma_a} \left( 1 + \varepsilon \xi_{n,i+\frac{1}{2}}^{l+\frac{1}{2}} \right) + D^{FD} \frac{q}{\Sigma_a} \left( \varepsilon \zeta_{i+1}^{l+\frac{1}{2}} - \varepsilon \zeta_i^{l+\frac{1}{2}} \right) \\
&\quad + \frac{1}{2} \sum_n w_n \mu_n \frac{q}{\Sigma_a} \frac{\varepsilon}{2} \left( \zeta_{i+1}^{l+1} + \zeta_i^{l+1} - \zeta_{i+1}^{l+\frac{1}{2}} - \zeta_i^{l+\frac{1}{2}} \right) + O(\varepsilon^2) \\
&= \frac{1}{2} \sum_n w_n \mu_n \frac{q}{\Sigma_a} \varepsilon \xi_{n,i+\frac{1}{2}}^{l+\frac{1}{2}} + D^{FD} \frac{q}{\Sigma_a} \left( \varepsilon \zeta_{i+1}^{l+\frac{1}{2}} - \varepsilon \zeta_i^{l+\frac{1}{2}} \right) + O(\varepsilon^2),
\end{aligned}$$

where  $\frac{1}{2} \sum_n w_n \mu_n = 0$  is considered in the last formulation.

Similarly, we have:

$$D_{i-\frac{1}{2}}^{cor,l+\frac{1}{2}}(\phi_i^{l+1} + \phi_{i-1}^{l+1}) = \frac{1}{2} \sum_n w_n \mu_n \frac{q}{\Sigma_a} \varepsilon \xi_{n,i-\frac{1}{2}}^{l+\frac{1}{2}} + D^{FD} \frac{q}{\Sigma_a} \left( \varepsilon \zeta_i^{l+\frac{1}{2}} - \varepsilon \zeta_{i-1}^{l+\frac{1}{2}} \right) + O(\varepsilon^2). \tag{18}$$

Substituting Eqs. (10), (17), and (18) into Eq.(8) and neglecting  $O(\varepsilon^2)$ , we have:

$$\begin{aligned}
& -D^{FD} \left( \frac{q}{\Sigma_a} (1 + \varepsilon \zeta_{i+1}^{l+1}) - \frac{q}{\Sigma_a} (1 + \varepsilon \zeta_i^{l+1}) \right) + \frac{1}{2} \sum_n w_n \mu_n \frac{q}{\Sigma_a} \varepsilon \xi_{n,i+\frac{1}{2}}^{l+\frac{1}{2}} \\
& \quad + D^{FD} \frac{q}{\Sigma_a} \left( \varepsilon \zeta_{i+1}^{l+\frac{1}{2}} - \varepsilon \zeta_i^{l+\frac{1}{2}} \right) \\
& \quad + D^{FD} \left( \frac{q}{\Sigma_a} (1 + \varepsilon \zeta_i^{l+1}) - \frac{q}{\Sigma_a} (1 + \varepsilon \zeta_{i-1}^{l+1}) \right) - \frac{1}{2} \sum_n w_n \mu_n \frac{q}{\Sigma_a} \varepsilon \xi_{n,i-\frac{1}{2}}^{l+\frac{1}{2}} \\
& \quad - D^{FD} \frac{q}{\Sigma_a} \left( \varepsilon \zeta_i^{l+\frac{1}{2}} - \varepsilon \zeta_{i-1}^{l+\frac{1}{2}} \right) + ph \Sigma_a \phi_i^{l+1} = phq.
\end{aligned} \tag{19}$$

By rearranging Eq.(19), we have:

$$\begin{aligned}
& -D^{FD} \left( \frac{q}{\Sigma_a} (\varepsilon \zeta_{i+1}^{l+1} - \varepsilon \zeta_i^{l+1}) \right) + \frac{1}{2} \sum_n w_n \mu_n \frac{q}{\Sigma_a} \left( \varepsilon \xi_{n,i+\frac{1}{2}}^{l+\frac{1}{2}} - \varepsilon \xi_{n,i-\frac{1}{2}}^{l+\frac{1}{2}} \right) \\
& \quad + D^{FD} \frac{q}{\Sigma_a} \left( \varepsilon \zeta_{i+1}^{l+\frac{1}{2}} - \varepsilon \zeta_i^{l+\frac{1}{2}} \right) + D^{FD} \left( \frac{q}{\Sigma_a} (\varepsilon \zeta_i^{l+1} - \varepsilon \zeta_{i-1}^{l+1}) \right) \\
& \quad - D^{FD} \frac{q}{\Sigma_a} \left( \varepsilon \zeta_i^{l+\frac{1}{2}} - \varepsilon \zeta_{i-1}^{l+\frac{1}{2}} \right) + ph \Sigma_a \frac{q}{\Sigma_a} (1 + \varepsilon \zeta_i^{l+1}) = phq, \\
& -D^{FD} (\zeta_{i+1}^{l+1} - \zeta_i^{l+1}) + \frac{1}{2} \sum_n w_n \mu_n \left( \xi_{n,i+\frac{1}{2}}^{l+\frac{1}{2}} - \xi_{n,i-\frac{1}{2}}^{l+\frac{1}{2}} \right) + D^{FD} \left( \zeta_{i+1}^{l+\frac{1}{2}} - \zeta_i^{l+\frac{1}{2}} \right) \\
& \quad + D^{FD} (\zeta_i^{l+1} - \zeta_{i-1}^{l+1}) - D^{FD} \left( \zeta_i^{l+\frac{1}{2}} - \zeta_{i-1}^{l+\frac{1}{2}} \right) + ph \Sigma_a \zeta_i^{l+1} = 0, \\
& -D^{FD} \zeta_{i+1}^{l+1} + 2D^{FD} \zeta_i^{l+1} - D_{i-\frac{1}{2}} \zeta_{i-1}^{l+1} + \frac{1}{2} \sum_n w_n \mu_n \left( \xi_{n,i+\frac{1}{2}}^{l+\frac{1}{2}} - \xi_{n,i-\frac{1}{2}}^{l+\frac{1}{2}} \right) + D^{FD} \zeta_{i+1}^{l+\frac{1}{2}} \\
& \quad - 2D^{FD} \zeta_i^{l+\frac{1}{2}} + D^{FD} \zeta_{i-1}^{l+\frac{1}{2}} + ph \Sigma_a \zeta_i^{l+1} = 0.
\end{aligned} \tag{20}$$

By integrating Eq.(1) with angle, we have:

$$\begin{aligned}
& \sum_n \mu_n w_n \frac{\psi_{n,k+\frac{1}{2}}^{l+\frac{1}{2}} - \psi_{n,k-\frac{1}{2}}^{l+\frac{1}{2}}}{h} + \sum_n \Sigma_t w_n \left( f_n \psi_{n,k+\frac{1}{2}}^{l+\frac{1}{2}} + (1 - f_n) \psi_{n,k-\frac{1}{2}}^{l+\frac{1}{2}} \right) \\
& \quad = \sum_n w_n (\Sigma_s \phi_k^l + q), \\
& \sum_n \mu_n w_n \frac{\psi_{n,k+\frac{1}{2}}^{l+\frac{1}{2}} - \psi_{n,k-\frac{1}{2}}^{l+\frac{1}{2}}}{h} + \sum_n \Sigma_t w_n \left( f_n \psi_{n,k+\frac{1}{2}}^{l+\frac{1}{2}} + (1 - f_n) \psi_{n,k-\frac{1}{2}}^{l+\frac{1}{2}} \right) = 2(\Sigma_s \phi_k^l + q), \\
& \frac{1}{2} \sum_n \mu_n w_n \frac{\psi_{n,k+\frac{1}{2}}^{l+\frac{1}{2}} - \psi_{n,k-\frac{1}{2}}^{l+\frac{1}{2}}}{h} + \frac{1}{2} \Sigma_t \sum_n w_n \left( f_n \psi_{n,k+\frac{1}{2}}^{l+\frac{1}{2}} + (1 - f_n) \psi_{n,k-\frac{1}{2}}^{l+\frac{1}{2}} \right) = \Sigma_s \phi_k^l + q,
\end{aligned} \tag{21}$$

$$\frac{1}{2} \sum_n \mu_n w_n \frac{\psi_{n,k+\frac{1}{2}}^{l+\frac{1}{2}} - \psi_{n,k-\frac{1}{2}}^{l+\frac{1}{2}}}{h} + \Sigma_t \phi_k^{l+\frac{1}{2}} = \Sigma_s \phi_k^l + q,$$

where Eq.(3) is used. Summing Eq.(21) for  $p$  fine cells consisting a coarse mesh of  $i$ , we have:

$$\begin{aligned} \frac{1}{2} \sum_n \mu_n w_n \frac{\psi_{n,i+\frac{1}{2}}^{l+\frac{1}{2}} - \psi_{n,i-\frac{1}{2}}^{l+\frac{1}{2}}}{h} + \Sigma_t \sum_k \phi_k^{l+\frac{1}{2}} &= \Sigma_s \sum_k \phi_k^l + \sum_k q, \\ \frac{1}{2} \sum_n \mu_n w_n \frac{\psi_{n,i+\frac{1}{2}}^{l+\frac{1}{2}} - \psi_{n,i-\frac{1}{2}}^{l+\frac{1}{2}}}{h} + \Sigma_t p \phi_i^{l+\frac{1}{2}} &= \Sigma_s p \phi_i^l + qp, \end{aligned} \quad (22)$$

where the following relations are used:

$$\begin{aligned} \phi_i^{l+\frac{1}{2}} &= \frac{1}{p} \sum_k \phi_k^{l+\frac{1}{2}}, \\ \phi_i^l &= \frac{1}{p} \sum_k \phi_k^l, \\ \sum_k q &= qp. \end{aligned} \quad (23)$$

Applying Eq.(10) to Eq.(23), we have:

$$\frac{1}{2} \sum_n \mu_n w_n \frac{\xi_{n,i+\frac{1}{2}}^{l+\frac{1}{2}} - \xi_{n,i-\frac{1}{2}}^{l+\frac{1}{2}}}{h} + \Sigma_t p \zeta_i^{l+\frac{1}{2}} = \Sigma_s p \zeta_i^l. \quad (24)$$

Substituting Eq.(24) to Eq.(20), we have:

$$\begin{aligned} -D^{FD} \zeta_{i+1}^{l+1} + 2D^{FD} \zeta_i^{l+1} - D^{FD} \zeta_{i-1}^{l+1} \\ + ph \Sigma_s \zeta_i^l - ph \Sigma_t \zeta_i^{l+\frac{1}{2}} \\ + D^{FD} \zeta_{i+1}^{l+\frac{1}{2}} - 2D^{FD} \zeta_i^{l+\frac{1}{2}} + D^{FD} \zeta_{i-1}^{l+\frac{1}{2}} + ph \Sigma_a \zeta_i^{l+1} = 0. \end{aligned} \quad (25)$$

Substituting Eq.(10) into Eq.(9), we have:

$$\begin{aligned} \frac{q}{\Sigma_a} (1 + \varepsilon \zeta_k^{l+1}) &= \frac{q}{\Sigma_a} \left( 1 + \varepsilon \zeta_k^{l+\frac{1}{2}} \right) \frac{\frac{q}{\Sigma_a} (1 + \varepsilon \zeta_i^{l+1})}{\frac{q}{\Sigma_a} (1 + \varepsilon \zeta_i^{l+\frac{1}{2}})}, \\ (1 + \varepsilon \zeta_k^{l+1}) &= \left( 1 + \varepsilon \zeta_k^{l+\frac{1}{2}} \right) \frac{(1 + \varepsilon \zeta_i^{l+1})}{(1 + \varepsilon \zeta_i^{l+\frac{1}{2}})}, \\ (1 + \varepsilon \zeta_k^{l+1}) &= \left( 1 + \varepsilon \zeta_k^{l+\frac{1}{2}} \right) \left( 1 + \varepsilon \zeta_i^{l+1} - \varepsilon \zeta_i^{l+\frac{1}{2}} + O(\varepsilon^2) \right), \end{aligned} \quad (26)$$



$$(1 + \varepsilon \zeta_k^{l+1}) = 1 + \varepsilon \zeta_i^{l+1} - \varepsilon \zeta_i^{l+\frac{1}{2}} + \varepsilon \zeta_k^{l+\frac{1}{2}} + O(\varepsilon^2),$$

$$\zeta_k^{l+1} = \zeta_k^{l+\frac{1}{2}} + \zeta_i^{l+1} - \zeta_i^{l+\frac{1}{2}} + O(\varepsilon).$$

Equations (25) and (26) represent the error by the CMFD equation.

### 2.3 Summary of angular flux and scalar flux errors in transport and CMFD equations

To sum up the derivation so far, Eqs.(27)-(30) are used to represent errors during transport iterations with the CMFD acceleration:

$$\mu_n \frac{1}{h \Sigma_t} \left( \xi_{n,k+\frac{1}{2}}^{l+\frac{1}{2}} - \xi_{n,k-\frac{1}{2}}^{l+\frac{1}{2}} \right) + \left( f_n \xi_{n,k+\frac{1}{2}}^{l+\frac{1}{2}} + (1 - f_n) \xi_{n,k-\frac{1}{2}}^{l+\frac{1}{2}} \right) = c \zeta_k^l, \quad (27)$$

$$\zeta_k^{l+\frac{1}{2}} = \frac{1}{2} \sum_n w_n \left( f_n \xi_{n,k+\frac{1}{2}}^{l+\frac{1}{2}} + (1 - f_n) \xi_{n,k-\frac{1}{2}}^{l+\frac{1}{2}} \right), \quad (28)$$

$$\begin{aligned} -D^{FD} \zeta_{i+1}^{l+1} + (2D^{FD} + ph \Sigma_a) \zeta_i^{l+1} - D^{FD} \zeta_{i-1}^{l+1} \\ + ph \Sigma_s \zeta_i^l - ph \Sigma_t \zeta_i^{l+\frac{1}{2}} \end{aligned} \quad (29)$$

$$+ D^{FD} \zeta_{i+1}^{l+\frac{1}{2}} - 2D^{FD} \zeta_i^{l+\frac{1}{2}} + D^{FD} \zeta_{i-1}^{l+\frac{1}{2}} = 0,$$

$$\zeta_k^{l+1} = \zeta_k^{l+\frac{1}{2}} + \zeta_i^{l+1} - \zeta_i^{l+\frac{1}{2}}. \quad (30)$$

### 2.4 Applying Fourier expansion to errors

Now we apply the Fourier expansion as follows:

$$\zeta_i^l = \omega^l A \exp(j \lambda x_i),$$

$$\zeta_k^l = \omega^l A_k \exp(j \lambda x_k),$$

$$\zeta_i^{l+\frac{1}{2}} = \omega^l B \exp(j \lambda x_i), \quad (31)$$

$$\zeta_k^{l+\frac{1}{2}} = \omega^l B_k \exp(j \lambda x_k),$$

$$\xi_{n,k+\frac{1}{2}}^{l+\frac{1}{2}} = \omega^l a_{n,k} \exp\left(j \lambda x_{k+\frac{1}{2}}\right),$$

where

$\omega$ : growth factor of error mode,

$A, B, A_k, B_k, a_{n,k}$ : expansion coefficients,

$\lambda$ : error mode frequency  $\times \Sigma_t$  in order to make  $\lambda x_i$  dimensionless,

$j$ : imaginary number,

$x_i$ : center position of coarse mesh  $i$ ,

$x_k$ : center position of fine mesh  $k$ ,

$x_{k+\frac{1}{2}}$ : position of boundary between fine meshes  $k$  and  $k+1$ .

## 2.5 Relation between $B_k$ and $A_k$ (express $B_k$ as a function of $A_k$ )

By substituting Eq.(31) into Eq.(27), we have:

$$\begin{aligned}
& \mu_n \frac{1}{h\Sigma_t} \left( \omega^l a_{n,k} \exp(j\lambda x_{k+\frac{1}{2}}) - \omega^l a_{n,k-1} \exp(j\lambda x_{k-\frac{1}{2}}) \right) \\
& \quad + \left( f_n \omega^l a_{n,k} \exp(j\lambda x_{k+\frac{1}{2}}) + (1-f_n) \omega^l a_{n,k-1} \exp(j\lambda x_{k-\frac{1}{2}}) \right) \\
& \quad = c \omega^l A_k \exp(j\lambda x_k), \\
& \mu_n \frac{1}{h\Sigma_t} (a_{n,k} \exp(j\lambda h) - a_{n,k-1}) + (f_n a_{n,k} \exp(j\lambda h) + (1-f_n) a_{n,k-1}) \\
& \quad = c A_k \exp\left(\frac{j\lambda h}{2}\right), \\
& \left(\frac{\mu_n}{h\Sigma_t} + f_n\right) \exp\left(\frac{j\lambda h}{2}\right) a_{n,k} + \left(-\frac{\mu_n}{h\Sigma_t} + 1 - f_n\right) \exp\left(-\frac{j\lambda h}{2}\right) a_{n,k-1} = c A_k,
\end{aligned} \tag{32}$$

where  $x_{k+\frac{1}{2}} - x_{k-\frac{1}{2}} = h$  is used.

Assuming the periodic boundary condition, Eq. (32) can be written as the matrix form. In the case of  $p=4$ :

$$\begin{aligned}
& \begin{bmatrix} \left(\frac{\mu_n}{h\Sigma_t} + f_n\right) e^{jv} & 0 & 0 & \left(-\frac{\mu_n}{h\Sigma_t} + 1 - f_n\right) e^{-jv} \\ \left(-\frac{\mu_n}{h\Sigma_t} + 1 - f_n\right) e^{-jv} & \left(\frac{\mu_n}{h\Sigma_t} + f_n\right) e^{jv} & 0 & 0 \\ 0 & \left(-\frac{\mu_n}{h\Sigma_t} + 1 - f_n\right) e^{-jv} & \left(\frac{\mu_n}{h\Sigma_t} + f_n\right) e^{jv} & 0 \\ 0 & 0 & \left(-\frac{\mu_n}{h\Sigma_t} + 1 - f_n\right) e^{-jv} & \left(\frac{\mu_n}{h\Sigma_t} + f_n\right) e^{jv} \end{bmatrix} \begin{bmatrix} a_{n,1} \\ a_{n,2} \\ a_{n,3} \\ a_{n,4} \end{bmatrix} \\
& = c \begin{bmatrix} A_1 \\ A_2 \\ A_3 \\ A_4 \end{bmatrix}.
\end{aligned} \tag{33}$$

where  $v = \frac{\lambda h}{2}$ . It should be noted that  $a_{n,0} = a_{n,4}$  because of the periodic boundary condition.

Substituting Eq.(31) into Eq. (28):

$$\begin{aligned} \omega^l B_k \exp(j\lambda x_k) &= \frac{1}{2} \sum_n w_n \left( f_n \omega^l a_{n,k} \exp\left(j\lambda x_{k+\frac{1}{2}}\right) \right. \\ &\quad \left. + (1 - f_n) \omega^l a_{n,k-1} \exp\left(j\lambda x_{k-\frac{1}{2}}\right) \right), \end{aligned} \quad (34)$$

$$B_k \exp\left(\frac{j\lambda h}{2}\right) = \frac{1}{2} \sum_n w_n (f_n a_{n,k} \exp(j\lambda h) + (1 - f_n) a_{n,k-1})$$

$$B_k = \frac{1}{2} \sum_n w_n f_n \exp\left(\frac{j\lambda h}{2}\right) a_{n,k} + \frac{1}{2} \sum_n w_n (1 - f_n) \exp\left(-\frac{j\lambda h}{2}\right) a_{n,k-1}.$$

Assuming the periodic boundary condition, Eq. (34) can be written as the matrix form. In the case of  $p=4$ :

$$\begin{bmatrix} B_1 \\ B_2 \\ B_3 \\ B_4 \end{bmatrix} = \frac{1}{2} \sum_n w_n \begin{bmatrix} f_n e^{jv} & 0 & 0 & (1 - f_n) e^{-jv} \\ (1 - f_n) e^{-jv} & f_n e^{jv} & 0 & 0 \\ 0 & (1 - f_n) e^{-jv} & f_n e^{jv} & 0 \\ 0 & 0 & (1 - f_n) e^{-jv} & f_n e^{jv} \end{bmatrix} \begin{bmatrix} a_{n,1} \\ a_{n,2} \\ a_{n,3} \\ a_{n,4} \end{bmatrix}. \quad (35)$$

Using Eqs.(33) and (35), we have:

$$\begin{aligned} \begin{bmatrix} B_1 \\ B_2 \\ B_3 \\ B_4 \end{bmatrix} &= \frac{c}{2} \sum_n w_n \begin{bmatrix} f_n e^{jv} & 0 & 0 & (1 - f_n) e^{-jv} \\ (1 - f_n) e^{-jv} & f_n e^{jv} & 0 & 0 \\ 0 & (1 - f_n) e^{-jv} & f_n e^{jv} & 0 \\ 0 & 0 & (1 - f_n) e^{-jv} & f_n e^{jv} \end{bmatrix} \times \\ &\begin{bmatrix} \left(\frac{\mu_n}{h\Sigma_t} + f_n\right) e^{jv} & 0 & 0 & \left(-\frac{\mu_n}{h\Sigma_t} + 1 - f_n\right) e^{-jv} \\ \left(-\frac{\mu_n}{h\Sigma_t} + 1 - f_n\right) e^{-jv} & \left(\frac{\mu_n}{h\Sigma_t} + f_n\right) e^{jv} & 0 & 0 \\ 0 & \left(-\frac{\mu_n}{h\Sigma_t} + 1 - f_n\right) e^{-jv} & \left(\frac{\mu_n}{h\Sigma_t} + f_n\right) e^{jv} & 0 \\ 0 & 0 & \left(-\frac{\mu_n}{h\Sigma_t} + 1 - f_n\right) e^{-jv} & \left(\frac{\mu_n}{h\Sigma_t} + f_n\right) e^{jv} \end{bmatrix}^{-1} \begin{bmatrix} A_1 \\ A_2 \\ A_3 \\ A_4 \end{bmatrix}. \end{aligned} \quad (36)$$

Equation (36) can be written as:

$$\mathbf{B} = \mathbf{H}\mathbf{A}, \quad (37)$$

where vectors  $\mathbf{A}$ ,  $\mathbf{B}$ , and matrix  $\mathbf{H}$  are given by:

$$\mathbf{A} = [A_1 \ A_2 \ A_3 \ A_4]^T, \quad (38)$$

$$\mathbf{B} = [B_1 \ B_2 \ B_3 \ B_4]^T,$$

$$\mathbf{H} = \frac{c}{2} \sum_n w_n \begin{bmatrix} f_n e^{j\nu} & 0 & 0 & (1-f_n)e^{-j\nu} \\ (1-f_n)e^{-j\nu} & f_n e^{j\nu} & 0 & 0 \\ 0 & (1-f_n)e^{-j\nu} & f_n e^{j\nu} & 0 \\ 0 & 0 & (1-f_n)e^{-j\nu} & f_n e^{j\nu} \end{bmatrix} \times$$

$$\begin{bmatrix} \left(\frac{\mu_n}{h\Sigma_t} + f_n\right) e^{j\nu} & 0 & 0 & \left(-\frac{\mu_n}{h\Sigma_t} + 1 - f_n\right) e^{-j\nu} \\ \left(-\frac{\mu_n}{h\Sigma_t} + 1 - f_n\right) e^{-j\nu} & \left(\frac{\mu_n}{h\Sigma_t} + f_n\right) e^{j\nu} & 0 & 0 \\ 0 & \left(-\frac{\mu_n}{h\Sigma_t} + 1 - f_n\right) e^{-j\nu} & \left(\frac{\mu_n}{h\Sigma_t} + f_n\right) e^{j\nu} & 0 \\ 0 & 0 & \left(-\frac{\mu_n}{h\Sigma_t} + 1 - f_n\right) e^{-j\nu} & \left(\frac{\mu_n}{h\Sigma_t} + f_n\right) e^{j\nu} \end{bmatrix}^{-1}.$$

In the case of  $p=2$ ,

$$\mathbf{A} = [A_1 \quad A_2]^T,$$

$$\mathbf{B} = [B_1 \quad B_2]^T,$$

$$\mathbf{H} = \frac{c}{2} \sum_n w_n \begin{bmatrix} f_n e^{j\nu} & (1-f_n)e^{-j\nu} \\ (1-f_n)e^{-j\nu} & f_n e^{j\nu} \end{bmatrix} \times \quad (39)$$

$$\begin{bmatrix} \left(\frac{\mu_n}{h\Sigma_t} + f_n\right) e^{j\nu} & \left(-\frac{\mu_n}{h\Sigma_t} + 1 - f_n\right) e^{-j\nu} \\ \left(-\frac{\mu_n}{h\Sigma_t} + 1 - f_n\right) e^{-j\nu} & \left(\frac{\mu_n}{h\Sigma_t} + f_n\right) e^{j\nu} \end{bmatrix}^{-1}.$$

In the case of  $p=1$ ,

$$\mathbf{A} = A_1,$$

$$\mathbf{B} = B_1,$$

$$\mathbf{H} = \frac{c}{2} \sum_n w_n \frac{[f_n e^{j\nu} + (1-f_n)e^{-j\nu}]}{\left(\frac{\mu_n}{h\Sigma_t} + f_n\right) e^{j\nu} + \left(-\frac{\mu_n}{h\Sigma_t} + 1 - f_n\right) e^{-j\nu}}. \quad (40)$$

Equation (40) can be split into the real and imaginary parts as follows when  $f_n = 1/2$ :

$$\begin{aligned}
\mathbf{H} &= \frac{c}{2} \sum_n w_n \frac{1}{1 + \frac{2\mu_n}{h\Sigma_t} \frac{e^{jv} - e^{-jv}}{e^{-jv} + e^{-jv}}} = \frac{c}{2} \sum_n w_n \frac{1}{1 + \frac{2\mu_n}{h\Sigma_t} j \tan v} \\
&= \frac{c}{2} \sum_n w_n \frac{1 - \frac{2\mu_n}{h\Sigma_t} j \tan v}{1 + \left(\frac{2\mu_n}{h\Sigma_t} \tan v\right)^2} \\
&= \frac{c}{2} \sum_n w_n \frac{1}{1 + \left(\frac{2\mu_n}{h\Sigma_t} \tan v\right)^2} - \frac{c}{2} \sum_n w_n \frac{\frac{2\mu_n}{h\Sigma_t} \tan v}{1 + \left(\frac{2\mu_n}{h\Sigma_t} \tan v\right)^2} j.
\end{aligned} \tag{41}$$

The real part of Eq. (41) corresponds to  $\kappa$  in Eq.(35) of Ref.[3], i.e., the derivation so far is consistent with those in Ref.[3].

## 2.5 Relation between $A_k$ and $B_k$ (express $A_k$ as a function of $B_k$ )

Substituting Eq.(31) into Eq.(29), we have:

$$\begin{aligned}
&-D^{FD} \omega^{l+1} A \exp(j\lambda x_{i+1}) + (2D^{FD} + ph\Sigma_\alpha) \omega^{l+1} A \exp(j\lambda x_i) \\
&\quad - D^{FD} \omega^{l+1} A \exp(j\lambda x_{i-1}) \\
&\quad + ph\Sigma_s \omega^l A \exp(j\lambda x_i) - ph\Sigma_t \omega^l B \exp(j\lambda x_i) \\
&+ D^{FD} \omega^l B \exp(j\lambda x_{i+1}) - 2D^{FD} \omega^l B \exp(j\lambda x_i) + D^{FD} \omega^l B \exp(j\lambda x_{i-1}) = 0, \\
&-D^{FD} \omega A \exp(j\lambda x_{i+1}) + (2D^{FD} + ph\Sigma_\alpha) \omega A \exp(j\lambda x_i) - D^{FD} \omega A \exp(j\lambda x_{i-1}) \\
&\quad + ph\Sigma_s A \exp(j\lambda x_i) - ph\Sigma_t B \exp(j\lambda x_i) \\
&+ D^{FD} B \exp(j\lambda x_{i+1}) - 2D^{FD} B \exp(j\lambda x_i) + D^{FD} B \exp(j\lambda x_{i-1}) = 0, \\
&-D^{FD} \omega A \exp(j\lambda ph) + (2D^{FD} + ph\Sigma_\alpha) \omega A - D^{FD} \omega A \exp(-j\lambda ph) \\
&\quad + ph\Sigma_s A - ph\Sigma_t B \\
&+ D^{FD} B \exp(j\lambda ph) - 2D^{FD} B + D^{FD} B \exp(-j\lambda ph) = 0.
\end{aligned} \tag{42}$$

In order to derive the third equation in Eq.(42), the both side of the second equation is divided by  $\exp(j\lambda x_i)$ , and the relation  $x_{i+1} - x_i = ph$  and  $x_{i-1} - x_i = -ph$  are used.

Similarly, from Eq.(30), we have the following relation:

$$\omega^{l+1} A_k \exp(j\lambda x_k) = \omega^l B_k \exp(j\lambda x_k) + \omega^{l+1} A \exp(j\lambda x_i) - \omega^l B \exp(j\lambda x_i), \tag{43}$$

$$\omega A_k \exp(j\lambda x_k) = B_k \exp(j\lambda x_k) + \omega A \exp(j\lambda x_i) - B \exp(j\lambda x_i).$$

From Eq. (43), we have:

$$\omega A - B = (\omega A_k - B_k) \frac{\exp(j\lambda x_k)}{\exp(j\lambda x_i)}. \quad (44)$$

From Eq.(42), we have:

$$\begin{aligned} & (-D^{FD} \exp(j\lambda ph) + (2D^{FD} + ph\Sigma_a) - D^{FD} \exp(-j\lambda ph))\omega A \\ & - (-D^{FD} \exp(j\lambda ph) + (2D^{FD} + ph\Sigma_a) - D^{FD} \exp(-j\lambda ph))B \\ & + ph\Sigma_s A - ph\Sigma_s B = 0, \quad (45) \\ & (-D^{FD} \exp(j\lambda ph) + (2D^{FD} + ph\Sigma_a) - D^{FD} \exp(-j\lambda ph))(\omega A - B) + ph\Sigma_s(A - B) \\ & = 0. \end{aligned}$$

Substituting Eq.(44) into Eq.(45), we have:

$$\begin{aligned} & (-D^{FD} \exp(j\lambda ph) + (2D^{FD} + ph\Sigma_a) - D^{FD} \exp(-j\lambda ph))(\omega A_k - B_k) \frac{\exp(j\lambda x_k)}{\exp(j\lambda x_i)} \\ & + ph\Sigma_s(A - B) = 0. \quad (46) \end{aligned}$$

Recall the definition of Eq.(23),

$$\begin{aligned} \phi_i^l &= \frac{1}{p} \sum_k \phi_k^l, \\ \phi_i^{l+\frac{1}{2}} &= \frac{1}{p} \sum_k \phi_k^{l+\frac{1}{2}}. \quad (47) \end{aligned}$$

Substituting Eqs.(10) and (31) into Eq.(47), we have:

$$\begin{aligned} A &= \frac{1}{p} \sum_k A_k \frac{\exp(j\lambda x_k)}{\exp(j\lambda x_i)}, \\ B &= \frac{1}{p} \sum_k B_k \frac{\exp(j\lambda x_k)}{\exp(j\lambda x_i)}. \quad (48) \end{aligned}$$

Therefore,

$$A - B = \frac{1}{p} \sum_k (A_k - B_k) \frac{\exp(j\lambda x_k)}{\exp(j\lambda x_i)}. \quad (49)$$

Substituting Eq.(49) into Eq.(46), we have:

$$\begin{aligned}
& (-D^{FD} \exp(j\lambda ph) + (2D^{FD} + ph\Sigma_a) - D^{FD} \exp(-j\lambda ph))(\omega A_k - B_k) \frac{\exp(j\lambda x_k)}{\exp(j\lambda x_i)} \\
& + ph\Sigma_s \frac{1}{p} \sum_{k'} (A_{k'} - B_{k'}) \frac{\exp(j\lambda x_{k'})}{\exp(j\lambda x_i)} = 0, \\
& (-D^{FD} \exp(j\lambda ph) + (2D^{FD} + ph\Sigma_a) - D^{FD} \exp(-j\lambda ph))(\omega A_k - B_k) \\
& + h\Sigma_s \sum_{k'} (A_{k'} - B_{k'}) \frac{\exp(j\lambda x_{k'})}{\exp(j\lambda x_k)} = 0.
\end{aligned} \tag{50}$$

Equation (50) can be rearranged as

$$\omega \mathbf{A} = -\theta \mathbf{W} \mathbf{A} + [\theta \mathbf{W} + \mathbf{I}] \mathbf{B}. \tag{51}$$

In the case of  $p=4$ :

$$\omega \begin{bmatrix} A_1 \\ A_2 \\ A_3 \\ A_4 \end{bmatrix} = \theta \mathbf{W} \begin{bmatrix} A_1 \\ A_2 \\ A_3 \\ A_4 \end{bmatrix} + [\theta \mathbf{W} + \mathbf{I}] \begin{bmatrix} B_1 \\ B_2 \\ B_3 \\ B_4 \end{bmatrix}, \tag{52}$$

where

$$\begin{aligned}
\theta &= \frac{h\Sigma_s}{(-D^{FD} \exp(j\lambda ph) + (2D^{FD} + ph\Sigma_a) - D^{FD} \exp(-j\lambda ph))} \\
&= \frac{h\Sigma_t c}{-D^{FD} (\cos 2pv + j \sin 2pv) + (2D^{FD} + ph\Sigma_t(1-c)) - D^{FD} (\cos 2pv - j \sin 2pv)} \\
&= \frac{h\Sigma_t c}{D^{FD} (2 - 2 \cos 2pv) + ph\Sigma_t(1-c)} = \frac{h\Sigma_t c}{4D^{FD} \sin^2 pv + ph\Sigma_t(1-c)}, \\
\mathbf{W} &= \begin{bmatrix} 1 & \exp(2jv) & \exp(4jv) & \exp(6jv) \\ \exp(-2jv) & 1 & \exp(2jv) & \exp(4jv) \\ \exp(-4jv) & \exp(-2jv) & 1 & \exp(2jv) \\ \exp(-6jv) & \exp(-4jv) & \exp(-2jv) & 1 \end{bmatrix}.
\end{aligned} \tag{53}$$

In the case of  $p=2$ ,

$$\omega \begin{bmatrix} A_1 \\ A_2 \end{bmatrix} = \theta \mathbf{W} \begin{bmatrix} A_1 \\ A_2 \end{bmatrix} + [\theta \mathbf{W} + \mathbf{I}] \begin{bmatrix} B_1 \\ B_2 \end{bmatrix}, \tag{54}$$

where

$$\begin{aligned}
\theta &= \frac{h\Sigma_t c}{4D^{FD} \sin^2 pv + ph\Sigma_t(1-c)}, \\
\mathbf{W} &= \begin{bmatrix} 1 & \exp(2jv) \\ \exp(-2jv) & 1 \end{bmatrix}.
\end{aligned} \tag{55}$$

In the case of  $p=1$ ,

$$\omega A_1 = \theta \mathbf{W} A_1 + [\theta \mathbf{W} + \mathbf{I}] B_1, \quad (56)$$

where

$$\theta = \frac{h \Sigma_t c}{4D^{FD} \sin^2 pv + ph \Sigma_t (1 - c)}, \quad (57)$$

$$\mathbf{W} = 1, \mathbf{I} = 1.$$

## 2.6 Iteration matrix for transport iteration with CMFD acceleration

Combining Eqs.(37) and (51), we finally obtain:

$$\omega \mathbf{A} = -\theta \mathbf{W} \mathbf{A} + [\theta \mathbf{W} + \mathbf{I}] \mathbf{H} \mathbf{A}, \quad (58)$$

$$\omega \mathbf{A} = [-\theta \mathbf{W} + [\theta \mathbf{W} + \mathbf{I}] \mathbf{H}] \mathbf{A}.$$

Thus, the iteration matrix is finally given by:

$$-\theta \mathbf{W} + [\theta \mathbf{W} + \mathbf{I}] \mathbf{H}. \quad (59)$$

The largest real eigenvalue of the matrix  $-\theta \mathbf{W} + [\theta \mathbf{W} + \mathbf{I}] \mathbf{H}$  dominates the convergence behavior of CMFD non-linear equation. If the absolute value of largest real eigenvalue exceeds 1.0, the CMFD acceleration diverges.

In the case of  $p=1$ ,  $\omega$  is simply given by:

$$-\theta + \theta \mathbf{H} + \mathbf{H}, \quad (60)$$

where  $\theta$  and  $\mathbf{H}$  are defined by Eq. (57) and the real part of Eq.(40), respectively.

In the case of  $p=4$ ,  $\mathbf{H}$ ,  $\mathbf{W}$ , and  $\theta$  are given by: Eqs.(53) and (38). In the case of  $p=2$ ,  $\mathbf{H}$ ,  $\mathbf{W}$ , and  $\theta$  are given by: Eqs.(55) and (39).