# Analyses of Sub-Cell Balance Methods with Linear Discontinuous Expansion for Three-Dimensional Discrete Ordinates Transport Equation

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### 1. Introduction

In this paper, two types of analyzes of two sub-cell balance methods (LDEM-SCB) which were implemented in the MUST (*M*ulti-group *U*nstructured geometry  $S_N$  *T*ransport) code[1] are performed for understanding of their computational characteristics. The first one is a numerical analysis to understand the convergence of the spatial differencing of the sub-cell methods[2,3] which are devised to solve three-dimensional discrete ordinates transport equation with tetrahedral meshes. The second one is the well-known asymptotic analysis in the thick diffusion limit to know if the sub-cell methods have the corresponding discretization schemes of diffusion equation in this limit.

## 2. Asymptotic Analysis in Thick Diffusion Limit

In thick diffusion limit[3], a spatial difference method is known to have good accuracy if the method has its corresponding accurate diffusion discretization including appropriate boundary conditions in this limit. Our analyses are done only for the problem interior. The analysis begins with the following scalings :

$$\sigma \to \sigma / \varepsilon, \sigma_a \to \varepsilon \sigma_a,$$
(1)  
$$\sigma_s \to \sigma / \varepsilon - \varepsilon \sigma_a, s \to \varepsilon s$$

where  $\varepsilon$  is a small parameter ( $\varepsilon \to 0$ ). Then the angular fluxes are expanded by the Talyor's series in this small parameter as follows :

$$\psi = \sum_{n=0}^{\infty} \psi^{(n)} \varepsilon^n.$$
 (2)

Then, Eq.(1) and Eq.(2) are substituted into the discretized one-group transport equation obtained by using the sub-cell balance methods with linear discontinuous expansion. After that, the coefficients for each power of  $\varepsilon$  are equated to obtain a hierarchy of equations. The integration of the equation for the coefficients of  $\varepsilon^{-1}$  over the directions leads to the fact that the leading-order angular flux  $\psi^{(0)}$  is isotropic. Some algebra show that the leading-order sub-cell average angular fluxes of LDEM-SCB(0) and LDEM-SCB(1)[2,3] are isotropic and so the leading point fluxes are isotropic because they can be represented in terms of the sub-cell average fluxes. Second, the

integration of the equations for the coefficients of  $\varepsilon^{0}$  over directions reveals the continuity of the leadingorder scalar fluxes. For LDEM-SCB(0), this equation says the continuity of the only face average leadingorder scalar fluxes while it says the continuity of the point leading-order scalar fluxes for LDEM-SCB(1). However, the continuity in LDEM-SCB(1) is valid if the incoming partial currents of the points is continuous. Next, the integration of the equation for the coefficients of  $\varepsilon^0$  over directions after multiplying it with  $\hat{\Omega}_{m}$  represents the first-order current in terms of the leading-order scalar fluxes (  $\phi^{(0)}$  ). Some algebraic manipulations show that both methods yield the desirable expressions for the first currents at points (or vertexes) that are exact for any linearly dependent leading-order scalar fluxes as in Ref. 4. This expression is given by

$$\vec{J}_{i}^{p(1)} = \frac{1}{3\sigma} \{ \frac{1}{3V} (\phi_{1}^{p(0)} \vec{A}_{1} + \phi_{2}^{p(0)} \vec{A}_{2} + \phi_{3}^{p(0)} \vec{A}_{3} + \phi_{4}^{p(0)} \vec{A}_{4}) \},$$
(3)

where *i* means a vertex point. Also, this expression means the first-order currents at four vertex points for each tetrahedral mesh are same. These first-order currents are accurate because the exact current is constant in a mesh with a linear trial space of the leading-order scalar flux. The final equation which leads to a contribution of a sub-cell to the discretized diffusion equation can be derived by integrating the equation for the coefficients of  $\varepsilon^{-1}$  over directions. For LDEM-SCB(0), this equation for the sub-cell 1 is given by

$$\begin{aligned} &-\frac{1}{3}\vec{A}_{l}\cdot(\vec{J}_{2}^{p(1)}+\vec{J}_{3}^{p(1)}+\vec{J}_{4}^{p(1)})+\sigma_{a^{1}}\frac{V}{4}[\frac{1}{16}\phi_{l}^{p(0)}+\frac{5}{16}(\phi_{2}^{p(0)}+\phi_{3}^{p(0)}+\phi_{4}^{p(0)})](5)\\ &=\frac{V}{4}[\frac{1}{16}s_{1}^{p(0)}+\frac{5}{16}(s_{2}^{p(0)}+s_{3}^{p(0)}+s_{4}^{p(0)})]+F(J_{p\pm}^{f(1)}),\end{aligned}$$

where the last term means the surface-average firstorder partial current terms. Then, Eq.(5) is transformed into the equation which is represented in terms of the surface average quantities because the leading-order point scalar fluxes are not continuous across the mesh faces. The resulting equation is the contribution of the sub-cell 1 to the discretized diffusion equation. This same procedure can be also applied to the corresponding sub-cell of the neighboring cell through the face 1. Then, the final discretized diffusion equation is obtained by adding these two equations and the firstorder partial current terms (i.e.,  $F(J_{p\pm}^{f(1)})$ ) are cancelled out during adding two equations.

The discretized diffusion equation for LDEM-SCB(1) can be derived by using a similar procedure described above while there is a different aspect that the final discretized diffusion equation is obtained by summing all the equations for all the sub-cells sharing a node and that the leading-order point scalar fluxes are the final unknown. For example, the contribution of sub-cell 1 of mesh k to the discretized diffusion equation is given by

$$\frac{13}{108}\vec{J}_{k,1}^{p(1)} \cdot \vec{A}_{1} + \frac{7}{108}(\vec{J}_{k,2}^{p(1)} + \vec{J}_{k,3}^{p(1)} + \vec{J}_{k,4}^{p(1)}) \cdot \vec{A}_{1} - \frac{2}{108}(\vec{J}_{k,2}^{p(1)} \cdot \vec{A}_{2} + \vec{J}_{k,3}^{p(1)} \cdot \vec{A}_{3} + \vec{J}_{k,4}^{p(1)} \cdot \vec{A}_{4}) + \frac{1}{144}[75\phi_{k,1}^{p(0)} + 23(\phi_{k,2}^{p(0)} + \phi_{k,3}^{p(0)} + \phi_{k,4}^{p(0)})]\sigma_{ak}\frac{V_{k}}{4} = \frac{1}{144}[75s_{k,1}^{p(0)} + 23(s_{k,2}^{p(0)} + s_{k,3}^{p(0)} + s_{k,4}^{p(0)})]\frac{V_{k}}{4} + F(J_{p\pm}^{f(1)}),$$

### 3. Convergence of Spatial Differences

This section numerically analyzes the order of convergence for the sub-cell balance methods as mesh refinement in the transport regime. For this purpose, we devised a test problem which is a simple cubic box. The problem size both in x- and y-directions changes depending on the z-direction mesh size (or number of zdirection meshes) while the z-direction problem size is fixed to 0.1cm. The boundary conditions both for x- and y-directions are all reflective while the ones for zdirection are vacuum. We used the following one-group cross sections :  $\sigma = 50cm^{-1}, \sigma_s = 49cm^{-1}$ . So, the mean free path is small (i.e., 0.02cm). Also, we considered an inhomogeneous source of 10#/cm<sup>3</sup>sec which is uniformly distributed in this problem. The seven levels of the mesh refinement are considered to check the order of the convergence. For all the levels, the problem is divided into cubic boxes and each cubic box is subdivided into six tetrahedrons. The number of cubic boxes for all the levels are fixed to 2 along the x- and ydirections  $(n_x=n_y=2)$  but the number of cubic boxes along the z-direction  $(n_z)$  for the levels 1, 2, 3, 4, 5, 6, and 7 are 2, 4, 8, 16, 32, 64, and 128, respectively. So, the side lengths  $(h_z)$  of the cubic box are  $0.1/n_z$ . Also, we set the x- and y-direction side lengths of the cubic boxes to be the same as  $h_z$ . We used the Chebyshev-Legendre quadrature set having 2(azimuthal) x2 (polar) directions per octant. Actually, the analytic solutions for each level of mesh refinement can be analytically obtained by solving one-dimensional  $S_4$  transport equation because this problem is actually onedimensional one in z-direction. We compared the pointwise L<sub>2</sub> norms of the errors in the scalar fluxes of LDEM-SCB(0) and -SCB(1) with those of DFEM (Discontinuous Finite Element Method)[4], the fully lumped DFEM and the mass lumped DFEM[3] in Fig. 1. This figure shows that LDEM-SCB(0) and -SCB(1) have the first and second-order convergences, respectively. As expected, it shows that LDEM-SCB(1)

has higher order of convergence that LDEM-SCB(0) and the fully lumped DFEM. Also, it is noted that the point-wise  $L_2$  norms of the errors of LDEM-SCB(1) is smaller than those of DFEM and the mass lumped DFEM for all the levels.



Fig. 1 Comparison of the  $L_2$  norm of errors as mesh refinement

#### 4. Summary and Conclusion

We performed the asymptotic thick diffusion limit and analyzed the order of convergence as mesh refinement in the transport regime for two-sub-cell balance methods. The results show that these sub-cell balance methods have thick diffusion limits and that LDEM-SCB(0) and -SCB(1) have the first and secondorder convergences, respectively. In particular, it is shown that LDEM-SCB(1) have smaller  $L_2$  norms of errors than DFEM in the test problem.

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