Linear Discontinuous Expansion-Based Sub-Cell Balance Difference Schemes for 3-D Unstructured Geometry S_N Transport Calculation

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1. Introduction

In this paper, two new sub-cell balance methods for discretizing the S_N transport equation using tetrahedral meshes are presented. The authors already have proposed a sub-cell balance method with the linear discontinuous flux expansion (LDEM-SCB)[1]. The method was found to give quite robust solutions in terms of positivity but its accuracy was degraded in the low flux regions in comparison with DFEM (Discontinuous Finite Element Method). The new sub-cell balance methods proposed in this paper is to improve the accuracy of the previously proposed LDEM-SCB. These methods are implemented in the MUST code[2].

2. Theory and Method

To devise new sub-cell balance methods, each tetrahedral mesh is divided into its four sub-cells which are shown in Fig. 1(b). The sub-cell division used in the previous LDEM-SCB is also shown in Fig. 1(a) for comparison. Main difference between two sub-cell divisions is the number of the external faces of each sub-cell. A sub-cell in the previous division has only one external face while the one in the new division has three external faces. New and the previous LDEM-SCBs use the linear discontinuous expansion of flux in each tetrahedral mesh. The final unknowns in LDEM-SCB are the sub-cell average fluxes. So, the internal faces and the external sub-faces average fluxes should be represented in terms of the four sub-cell average fluxes. The derivations of these relations are tedious and long, and so the only final results are given in this paper. The six internal face average fluxes are represented in terms of the sub-cell average fluxes as follows :

$$\psi_{m,if,\alpha,\beta} = 29/52(\psi_{m,s\alpha} + \psi_{m,s\beta}) - 3/52(\psi_{m,s\gamma} + \psi_{m,s\delta}), \quad (1)$$

where $\psi_{m,if,\alpha,\beta}$ is the internal face average flux between the sub-cells α and β. $\psi_{m,s\alpha}$ is the average flux for the sub-cell α. Similarly, the twelve external sub-face average fluxes are given by

$$\psi_{m,ef,\alpha,\beta} = 65/52\psi_{m,s\alpha} - 23/52\psi_{m,s\beta} + 5/52(\psi_{m,s\gamma} + \psi_{m,s\delta}), \quad (2)$$

where $\psi_{m,ef,\alpha,\beta}$ is the average flux over the external face which includes a node α and is on the external face β (see Fig. 1(b)). The sub-cell balance equations are obtained by integrating the S_N transport equation over the sub-cells. For example, the sub-cell equation over a subcell 1 is given by

$$\begin{aligned}&\frac{1}{3}\vec{A}_3\cdot\hat{\Omega}_m\psi_{m,ef,1,3} + \frac{1}{3}\vec{A}_2\cdot\hat{\Omega}_m\psi_{m,ef,1,2} + \frac{1}{3}\vec{A}_4\cdot\hat{\Omega}_m\psi_{m,ef,1,4} \\ &+ \vec{A}_{1,2}\cdot\hat{\Omega}_m\psi_{m,if,1,2} + \vec{A}_{1,4}\cdot\hat{\Omega}_m\psi_{m,if,1,4} + \vec{A}_{1,3}\cdot\hat{\Omega}_m\psi_{m,if,1,3} \\ &+ \sigma\psi_{m,s1}V_{s1} = q_{m,s1}V_{s1},\end{aligned} \quad (3)$$

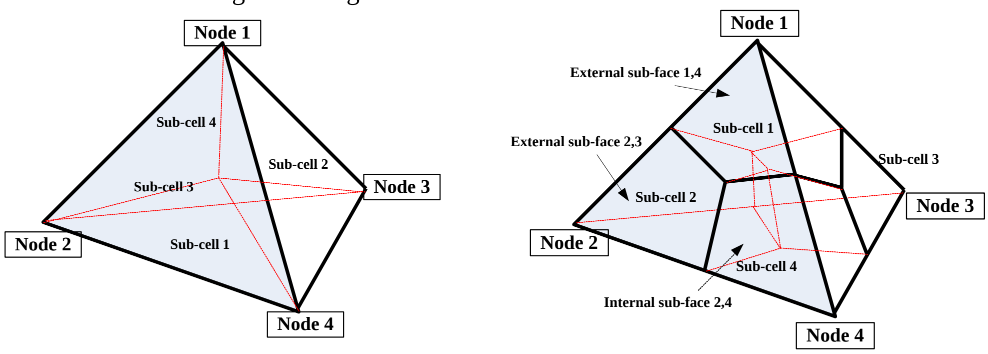
where $\vec{A}_\alpha$ is the outward normal vector whose magnitude is the area of the external face α, and $\vec{A}_{\alpha,\beta}$ is the outward normal vector which directs from the sub-cell α to β and its magnitude is the area of the interface face between the sub-cells α and β. In Eq.(3), V_{s1} and $q_{m,s1}$ is the volume and source of the sub-cell 1, respectively. The final form of the sub-cell balance equation is obtained by substituting Eq.(1) and (2) into Eq.(3). This equation is given by

$$\begin{aligned}&[\frac{65}{156}\{(1-\lambda)(\vec{A}_2+\vec{A}_3+\vec{A}_4)+\lambda(\delta_{2m}^O\vec{A}_2+\delta_{3m}^O\vec{A}_3+\delta_{4m}^O\vec{A}_4)\}\cdot\hat{\Omega}_m \\ &+\frac{29}{156}\vec{A}_1\cdot\hat{\Omega}_m+\sigma V_{s1}]\psi_{m,s1} \\ &+[\frac{5}{156}\vec{A}_1\cdot\hat{\Omega}_m-\{\frac{23}{156}(1-\lambda+\lambda\delta_{2m}^O)+\frac{8}{156}\}\vec{A}_2\cdot\hat{\Omega}_m \\ &+\frac{5}{156}\{(1-\lambda)(\vec{A}_3+\vec{A}_4)+\lambda(\delta_{3m}^O\vec{A}_3+\delta_{4m}^O\vec{A}_4)\}\cdot\hat{\Omega}_m]\psi_{m,s2} \\ &+[\frac{5}{156}\vec{A}_1\cdot\hat{\Omega}_m-\{\frac{23}{156}(1-\lambda+\lambda\delta_{3m}^O)+\frac{8}{156}\}\vec{A}_3\cdot\hat{\Omega}_m \\ &+\frac{5}{156}\{(1-\lambda)(\vec{A}_2+\vec{A}_4)+\lambda(\delta_{2m}^O\vec{A}_2+\delta_{4m}^O\vec{A}_4)\}\cdot\hat{\Omega}_m]\psi_{m,s3} \\ &+[\frac{5}{156}\vec{A}_1\cdot\hat{\Omega}_m-\{\frac{23}{156}(1-\lambda+\lambda\delta_{4m}^O)+\frac{8}{156}\}\vec{A}_4\cdot\hat{\Omega}_m \\ &+\frac{5}{156}\{(1-\lambda)(\vec{A}_2+\vec{A}_3)+\lambda(\delta_{2m}^O\vec{A}_2+\delta_{3m}^O\vec{A}_3)\}\cdot\hat{\Omega}_m]\psi_{m,s4} \\ &=q_{m,s1}V_{s1}-\frac{1}{3}(1-\delta_{2m}^O)\lambda\vec{A}_2\cdot\hat{\Omega}_m\psi_{m,exf,1,2}^{upc}-\frac{1}{3}(1-\delta_{3m}^O)\lambda\vec{A}_3\cdot\hat{\Omega}_m\psi_{m,exf,1,3}^{upc} \\ &-\frac{1}{3}(1-\delta_{4m}^O)\lambda\vec{A}_4\cdot\hat{\Omega}_m\psi_{m,exf,1,4}^{upc}.\end{aligned} \quad (4)$$

In Eq.(4), $\delta_{\alpha,m}^o$ is unity only if $\vec{A}_\alpha\cdot\hat{\Omega}_m > 0$ and $\psi_{m,exf,\alpha,\beta}^{upc}$ is the incoming flux over a external sub-face from the upcoming cell. The sub-cell balance method[3] is denoted as LDEM-SCB(1). The four sub-cell balance equations comprise a 4x4 matrix equation. After this 4x4 equation is solved, the outgoing external sub-face fluxes are calculated by Eq.(2) and they are used as the incoming sub-face fluxes in the adjacent cells. Another sub-cell method denoted by LDEM-SCB(2) is obtained by simply replacing the external sub-face average fluxes with the external face average ones in the right hand side of Eq.(5). Obviously, this method will have lower accuracy than LDEM-SCB(1) because the fewer flux information come from the upcoming cells.

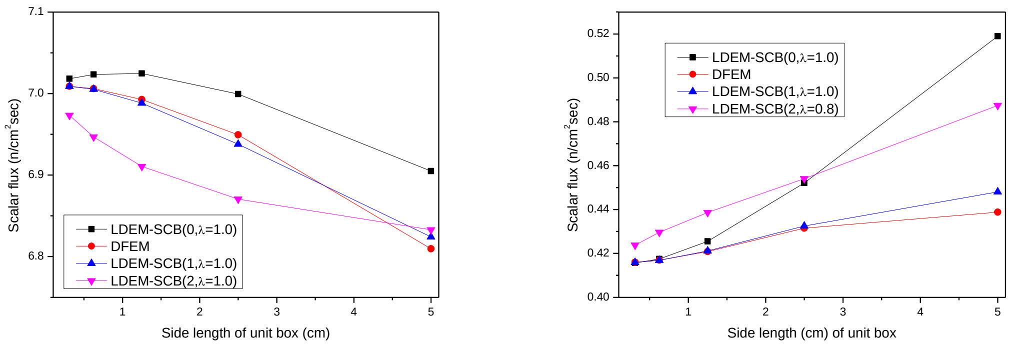
3. Numerical and Discussion

In this section, new sub-cell balance methods are tested for the box problem which is given in Ref. 1. This problem is defined by [0<x<20cm], [0<y<5cm], and [0<z<5cm]. The boundary conditions are vacuums on the external boundaries. This problem is divided into four coarse cubic regions of equal volume in x-direction. These four regions are numbered by 1, 2, 3, and 4 such that the region 1 is leftmost and the region 4 is rightmost along x-axis. This problem is a one-group fixed source problem. The homogeneous fixed neutron sources of 10.0 and 5.0 n/cm^{3}sec are given in the regions 1 and 2, respectively. The Chebyshev-Legendre angular quadrature used in this calculation has 2 polar angles and 2 azimuthal angles per an octant. For this problem, the five different cases of mesh divisions are considered to assess the accuracy of LDEM-SCB. The first, second, third, fourth, and fifth cases divide the problem into 24, 192, 1536, 12288, and 98304 tetrahedrons of equal volume, respectively. They correspond to 5cm, 2.5cm, 1.25cm, 0.625cm, and 0.3125cm side lengths of a unit cubic box, respectively. One unit cubic box consists of six tetrahedral meshes of equal volume.



(a) Old division (b) New division

Fig. 1 Comparison of the sub-cell divisions



(a) Region 2 (b) Region 3

Fig. 2 Comparison of the region average scalar fluxes versus of side length of the unit box.

Fig. 2(a) and 2(b) compares the region 2 and 3 average scalar fluxes over the side length of an unit box, respectively. These figures show that LDEM-SCB(2) gives quite accurate solutions in comparison with DFEM while the solution of LDEM-SCB(1) is not so accurate and slow convergence versus the side length of the unit box. However, it was found that LDEM-SCB(0) and LDEM-SCB(2) give more robust solutions in terms of positivity than DFEM and LDEM-SCB(1).

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