A Comparison of Two Spatial Difference Schemes with an Unstructured Triangular Mesh for a Two-Dimensional Geometry

Jong Woon Kim*, Ser Gi Hong, and Young-Ouk Lee
Korea Atomic Energy Research Institute, 1045 Daedeokdaero, Yuseong-gu, Daejeon, Korea, 305-353
**Corresponding author: jwkim@kaeri.re.kr*

1. Introduction

Solutions for the neutron transport equation are obtained most often by the discrete ordinates method, often referred to as the S_N method. A number of computer codes have been developed using the S_N method in rectangular, cylindrical or spherical geometry.

The use of such a specific regular mesh leads to the simplest difference equations but may require an excessive number of mesh points to describe complicated geometries adequately.

An unstructured triangular mesh is a good compromise because it is flexible enough to represent the complicated geometries.

The objective of this paper is to compare the accuracy of two spatial difference schemes (diamond difference-like and step characteristic schemes) with a two-dimensional unstructured triangular mesh.

2. Method and results

2.1 Derivation of the Governing Equation

The discrete ordinates equation in x-y geometry is

$$\left[\mu_m \frac{\partial}{\partial x}+\eta_m \frac{\partial}{\partial y}+\sigma_t(x,y)\right]\psi_m(x,y) = q_m(x,y), \qquad (1)$$

where m is the ordinate index.

Eq. (1) can be rewritten in operator form as follow:

$$\nabla\bullet\hat{\Omega}_m\psi_m + \sigma_t\psi_m = q_m. \qquad (2)$$

After integrating Eq. (2) over a triangular cell, using the divergence theorem to express the volume integral as a surface integral for the first term of Eq. (2) gives

$$\begin{aligned}&\hat{\Omega}_m\bullet\hat{n}_{1,k}\int_{S_{1,k}}\psi_m\,ds + \hat{\Omega}_m\bullet\hat{n}_{2,k}\int_{S_{2,k}}\psi_m\,ds\\ &+\hat{\Omega}_m\bullet\hat{n}_{3,k}\int_{S_{3,k}}\psi_m\,ds + \sigma_t\int_{V_k}\psi_m\,dv = \int_{V_k} q_m\,dv,\end{aligned} \qquad (3)$$

where $\hat{n}_1$, $\hat{n}_2$ and $\hat{n}_3$ are unit outward normal vectors, k is cell index and V_k is the volume of k cell.

We make the following definitions

$$\begin{aligned}&\psi_{1,m,k} \equiv \int_{S_{1,k}}\psi_m\,ds \Big/ S_{1,k}, \quad \psi_{2,m,k} \equiv \int_{S_{2,k}}\psi_m\,ds \Big/ S_{2,k},\\ &\psi_{3,m,k} \equiv \int_{S_{3,k}}\psi_m\,ds \Big/ S_{3,k}, \quad \psi_{0,m,k} \equiv \int_{V_k}\psi_m\,dv \Big/ V_k,\\ &q_{0,m,k} \equiv \int_{V_k} q_m\,dv \Big/ V_k, \quad A_{1,m,k} \equiv \left(\hat{\Omega}_m\bullet\hat{n}_1\,S_{1,k}\right),\\ &A_{2,m,k} \equiv \left(\hat{\Omega}_m\bullet\hat{n}_2\,S_{2,k}\right), \quad A_{3,m,k} \equiv \left(\hat{\Omega}_m\bullet\hat{n}_3\,S_{3,k}\right),\end{aligned} \qquad (4)$$

to obtain

$$\begin{aligned}&A_{1,m,k}\psi_{1,m,k} + A_{2,m,k}\psi_{2,m,k} + A_{3,m,k}\psi_{3,m,k}\\ &+\sigma_t\psi_{0,m,k}V_k = q_{0,m,k}V_k.\end{aligned} \qquad (5)$$

2.2 Diamond Difference-Like (DD-like) Scheme

This scheme is suggested by W. H. Reed [1] and it has a second order accuracy. This scheme uses the approximation that the cell-average flux is the average of the cell-face fluxes and the cell-face fluxe is the average of the two vertex fluxes.

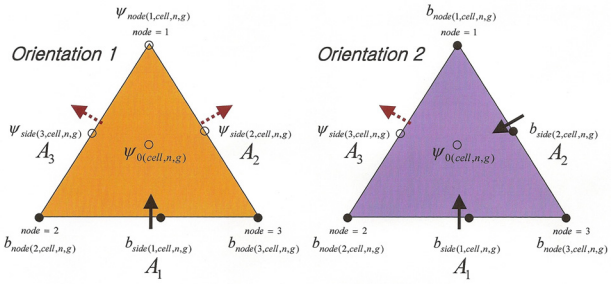

Fig. 1. Two orientations of triangles (DD-like scheme).

The two possible orientations of a triangle with respect to a direction $\hat{\Omega}_m$ are shown in Fig. 1. The b and ψ represent known and unknown fluxes, respectively. With some algebra, the resulting equations for two orientations are

Orientation 1:

$$\begin{aligned}&\psi_0 = \frac{q_0 V+\left(\frac{A_2+A_3}{2}-A_1\right)b_{side(1)}+\left(\frac{A_2-A_3}{4}\right)b_{node(2)}+\left(\frac{A_3-A_2}{4}\right)b_{node(3)}}{\left(\frac{3A_2}{2}+\frac{3A_3}{2}+\sigma_t V\right)},\\ &\psi_{node(1)} = 3\psi_0 - \frac{b_{node(2)}}{2} - \frac{b_{node(3)}}{2} - b_{side(1)},\\ &\psi_{side(2)} = \frac{b_{node(3)}+\psi_{node(1)}}{2},\\ &\psi_{side(3)} = \frac{b_{node(2)}+\psi_{node(1)}}{2},\end{aligned} \qquad (6)$$

Orientation 2:

$$\begin{aligned}&\psi_0 = \frac{q_0 V+(A_3-A_1)b_{side(1)}+(A_3-A_2)b_{side(2)}}{(3A_3+\sigma_t V)},\\ &\psi_{side(3)} = 3\psi_0 - b_{side(1)} - b_{side(2)}.\end{aligned} \qquad (7)$$

2.3 Step Characteristic (SC) Scheme

In the step characteristic scheme, the outgoing edge fluxes are calculated by integrating the characteristic form of Eq. (2) while the flat source distribution is assumed on the cell interior.

The two configurations of triangles are shown in Fig. 2 and the resulting equations for each orientation are given in Eqs. (8) and (9).

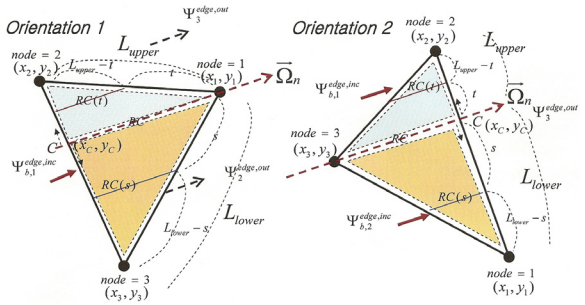

Fig. 2. Two orientations of triangles (SC scheme).

Orientation 1:

$$\Psi_3^{edge,out} = \frac{q_0}{\sigma_t} + \left(\frac{\kappa_n}{\sigma_t \overline{RC}}\right)\left(1-e^{\left(-\frac{\sigma_t \overline{RC}}{\kappa_n}\right)}\right)\left(\Psi_{b,1}^{edge,inc} - \frac{q_0}{\sigma_t}\right),$$

$$\Psi_2^{edge,out} = \frac{q_0}{\sigma_t} + \left(\frac{\kappa_n}{\sigma_t \overline{RC}}\right)\left(1-e^{\left(-\frac{\sigma_t \overline{RC}}{\kappa_n}\right)}\right)\left(\Psi_{b,1}^{edge,inc} - \frac{q_0}{\sigma_t}\right), \quad (8)$$

$$\Psi_0 = \frac{q_0 V - A_1\Psi_{b,1}^{edge,inc} - A_2\Psi_2^{edge,out} - A_3\Psi_3^{edge,out}}{\sigma_t V},$$

Orientation 2:

$$\Psi_3^{edge,out} = \frac{q_0}{\sigma_t} + \left(\frac{\kappa_n}{\sigma_t \overline{RC}}\right)\left(1-e^{\left(-\frac{\sigma_t \overline{RC}}{\kappa_n}\right)}\right)\left(\frac{\left(L_{upper}\Psi_{b,1}^{edge,inc} + L_{lower}\Psi_{b,2}^{edge,inc}\right)}{\left(L_{upper}+L_{lower}\right)} - \frac{q_0}{\sigma_t}\right), \quad (9)$$

$$\Psi_0 = \frac{q_0 V - A_1\Psi_{b,1}^{edge,inc} - A_2\Psi_{b,2}^{edge,inc} - A_3\Psi_3^{edge,out}}{\sigma_t V},$$

where $\kappa_n = \sqrt{1-\xi_n^2}$.

2.4 Test and Results

For verification, the test problem is configured as shown in Fig. 3 (circle, triangle, cross, and inner-square are embedded in the 7cm×7cm big outer-square).

The unstructured triangular mesh is generated by Triangle [2] code. The cross-sections and parameters are listed in Table I. The reference k_{eff} is calculated by MCNP5 [3] with the identical two group cross-section data.

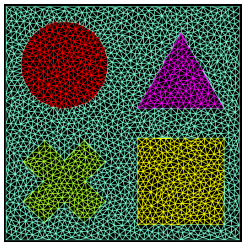

Fig. 3. Unstructured triangular mesh for test problem I.

The four regions which consist of mat1 (U^{235}) are surrounded by mat2 (H_2O) with a vacuum boundary condition. The macroscopic cross-sections for each region can be obtained by multiplying density multiplier to the cross-sections in Table I.

Table I: Cross-sections and parameters

# of cell	3049	
	mat1 (barn)	mat2 (cm^{-1})
$\sigma_{tot,1}$	2.23324e+2	1.57862e+0
$\nu\sigma_{f,1}$	4.20400e+2	-
$\sigma_{s,1\to1}$	1.42000e+1	6.41100e-1
$\sigma_{s,1\to2}$	1.24300e-1	9.30400e-1
$\sigma_{tot,2}$	2.75497e+3	6.42604e+0
$\nu\sigma_{f,2}$	5.61700e+3	-
$\sigma_{s,2\to1}$	-	-
$\sigma_{s,2\to2}$	1.59700e+1	6.34300e+0
density multiplier	circle: 0.03410 triangle: 0.04894 cross: 0.04850 inner-square: 0.03114	outer-square: 1.0

In the Table II, the k_{eff} results with two spatial difference schemes are compared. We find that the k_{eff} of the DD-like scheme is about one order better than that of the SC scheme. The scalar flux of the 2nd group with DD-like scheme is shown in Fig. 4.

Table II: The k_{eff} results

Reference (MCNP5): 1.98499±0.00001				
	DD-like		SC	
S_N order	k_{eff}	Difference (pcm) †	k_{eff}	Difference (pcm)
2	1.98352	-147	1.97987	-512
4	1.98470	-29	1.98136	-363
6	1.98475	-24	1.98146	-353
8	1.98477	-22	1.98151	-348
10	1.98479	-20	1.98153	-346
12	1.98479	-20	1.98154	-345
14	1.98480	-19	1.98155	-344
16	1.98480	-19	1.98155	-344
18	1.98481	-18	1.98155	-344
20	1.98483	-16	1.98156	-343

†Difference (pcm) = $(k_{eff} - k_{eff}(\text{reference}))\times10^5$

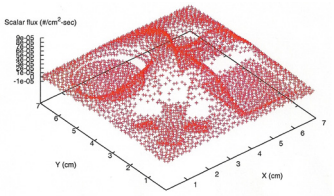

Fig. 4. The scalar flux of the 2nd group (DD-like scheme, S_{16}).

3. Conclusions

The k_{eff} results with two spatial difference schemes in an unstructured triangular mesh are presented and compared for the reference MCNP5 calculation.

The numerical test shows that two schemes implemented in an unstructured triangular mesh give accurate solution. The DD-like scheme shows better results than the SC scheme, even though there is still the possibility to need a negative flux fixup.

Acknowledgement

This work is supported by Agency for Defense Development (Contract No. UC080023GD).

REFERENCES

[1] W. H. Reed, Triangular Mesh Difference Schemes for the Transport Equation, LA-4769, Los Alamos National Laboratory, 1971.

[2] J. R. Shewchuk, "Triangle: A Two-Dimensional Quality Mesh Generator and Delaunay Triangulator," 2005. URL http://www.cs.cmu.edu/~quake/triangle.html

[3] X-5 Monte Carlo Team, "MCNP – A General Monte Carlo N-Particle Transport Code, Version 5, Volume I, II, III," LA-CP-03-0245, Los Alamos National Laboratory, 2003.