Implementation and Verification of adjoint neutron transport calculation in MUST code

Ta Duy Long, Ser Gi Hong*
Dept. Of Nuclear Engineering, Hanyang University, 222 Wangsimni-ro, Seongdong-gu, Seoul, Korea
**Corresponding author: hongsergi@hanyang.ac.kr*

1. Introduction

The adjoint solution of the Boltzmann neutron transport equation has been known as the importance of the neutrons to a response within a particular system [1] and the adjoint solution or flux is widely used in reactor analysis where the sensitivity calculations are performed with the perturbation theory. Also, in shielding design analysis, the adjoint flux has an important role because it can be used with variance reduction technique.

The objective of this work is to implement and verify an option for adjoint transport calculation in the MUST code [2, 3], which is a deterministic transport code using tetrahedral meshes for complicated geometrical problems. In particular, the adjoint calculation was performed with a small change of the forward transport calculation procedure. The adjoint solution obtained by MUST code calculation for a fixed source problem was verified by showing that the detector response calculated by the forward neutron flux is the same as the one obtained with the adjoint flux and the external forward source while the adjoint solution for eigenvalue problem was by showing that the forward and adjoint eigenvalues are same each other. Furthermore, the neutron fluxes in these verification problems were compared with the results calculated by using PARTISN code [4].

2. Theory and Methods

In this section, the adjoint transport equation is reviewed and the procedure for adjoint flux calculation is described. The starting equation is the adjoint transport equation with an external source, which is given by

$$-\hat{\Omega}.\nabla\psi^{+}(r,E,\hat{\Omega})+\sigma_t(r,E)\psi^{+}(r,E,\hat{\Omega})=\int_0^{\infty}dE'\int_{4\pi}d\hat{\Omega}'\,\sigma_s(r,E\to E',\hat{\Omega}.\hat{\Omega}')\psi^{+}(r,E',\hat{\Omega}')+S^{+}(r,E,\hat{\Omega}). \quad (1)$$

For the vacuum boundary condition, the adjoint angular fluxes for outgoing directions are zero, and so the adjoint calculation with sweeping is started from the opposite directions in comparison with the forward transport. To explain how we can use the forward transport calculation procedure for adjoint flux, we rewrite Eq. (1) by replacing $-\hat{\Omega}$ with a new angular variable $\hat{\Omega}$ where the new variable is the same as in the forward solution as follows:

$$\hat{\Omega}.\nabla\psi^{+}(r,E,-\hat{\Omega})+\sigma_t(r,E)\psi^{+}(r,E,-\hat{\Omega})=\int_0^{\infty}dE'\int_{4\pi}d\hat{\Omega}'\,\sigma_s(r,E\to E',-\hat{\Omega}.\hat{\Omega}')\psi^{+}(r,E',\hat{\Omega}')+S^{+}(r,E,-\hat{\Omega}). \quad (2)$$

The left hand side of Eq. (2) is actually the same form as that of the forward transport equation, except that the angular flux is at the opposite direction ($-\hat{\Omega}$). The scattering cross section in the right hand side of Eq. (2) can be expanded by using Legendre polynomial and the additional theorem of spherical harmonics as

$$\sigma_s(r,E\to E',-\hat{\Omega}.\hat{\Omega}')=\sum_{l=0}^{L}(2l+1)\,\sigma_{sl}(r,E\to E')\,[P_l(\mu)P_l(\mu')+\sum_{m=1}^{l}Y_{lm}^{e}(\hat{\Omega})\,Y_{lm}^{e}(\hat{\Omega}')-\sum_{m=1}^{l}Y_{lm}^{o}(\hat{\Omega})\,Y_{lm}^{o}(\hat{\Omega}')]. \quad (3)$$

It can be seen from Eq. (3) that the differences between scattering source terms in the adjoint and forward transport equations are the arrow direction in energy transfer by scattering cross-section and the sign of the odd parity spherical harmonic term. The flux moments in adjoint calculation are defined by

$$\phi_l^{+}(r,E)=\int_{4\pi}d\hat{\Omega}\,P_l(\mu)\psi^{+}(r,E,-\hat{\Omega}),$$

$$\phi_{lm}^{+,e}(r,E)=\int_{4\pi}d\hat{\Omega}\,Y_{lm}^{e}(\hat{\Omega})\psi^{+}(r,E,-\hat{\Omega}),$$

and

$$\phi_{lm}^{+,o}(r,E)=\int_{4\pi}d\hat{\Omega}\,Y_{lm}^{o}(\hat{\Omega})\psi^{+}(r,E,-\hat{\Omega}). \quad (4)$$

The flux moments in Eq. (4) are updated using the angular flux at the opposite direction ($-\hat{\Omega}$) because it is the result of Eq. (2). By using the odd moment of adjoint flux given by Eq. (4), the negative sign of the odd parity spherical harmonic in Eq. (3) can be removed. Finally, the form of adjoint transport equation without fission source is given by

$$\hat{\Omega}.\nabla\psi^{+}(r,E,-\hat{\Omega})+\sigma_t(r,E)\psi^{+}(r,E,-\hat{\Omega})= \sum_{l=0}^{L}(2l+1)\int_0^{\infty}dE'\,\sigma_{sl}(r,E\rightarrow E')[P_l(\mu)\phi_l^{+}(r,E') +\sum_{m=1}^{l}Y_{lm}^{e}(\hat{\Omega})\,\phi_{lm}^{+,e}(r,E') +\sum_{m=1}^{l}Y_{lm}^{o}(\hat{\Omega})\,\phi_{lm}^{+,o}(r,E')] +S^{+}(r,E,-\hat{\Omega}). \quad (5)$$

Therefore, the adjoint transport equation is very similar to the forward transport equation if the scattering cross section matrix is transposed. The within group calculation for the adjoint flux can be solved by the same procedure as in the forward calculation. The scattering source can be updated after each iteration using the angular adjoint flux in opposite direction as presented in Eq. (4). For eigenvalue problems, the fission source is added to Eq. (5) as follows:

$$q_f(r,E)=\nu\sigma_f(r,E)\int_0^{\infty}dE'\,\chi(E')\phi^{+}(r,E'). \quad (6)$$

As shown in Eq. (6), the fission source term in the adjoint equation is also similar to that in the forward transport equation with replacement of the fission cross-section with the fission yield in each neutron group. Finally, the order of the energy group sweeping should be reversed for the efficient calculation.

3. Verification of Adjoint Solution

4.1. Fixed source problem

For verification of adjoint transport calculation with fixed source problem, we considered a simple test problem which has the sizes of 9 cm x 5 cm x 1 cm in x-, y- and z-direction, respectively. This problem can be considered as a 2-D problem due to reflective boundary conditions in z-direction. In particular, we considered a small size problem to avoid the spatial truncation errors that makes it difficult to perform verification by comparing with other codes. The problem description is given in Fig. 1, where the reflective condition was used in the left boundary.

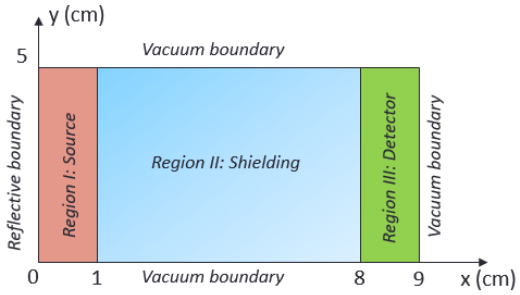

Fig.1 Fixed source problem description

In this problem, the leftmost region (region I) of 1 cm thickness in x-direction has a uniform source of 100 n/cm^2.s in the first ten neutron groups. We assumed that this region is composed of UO_2 (4.5 wt% enriched uranium). The next 7 cm thick region was considered as a shielding region composed of ^{56}Fe with a density of 7.87 g/cm^3. The last 1cm thick region was considered as a detector region composed of UO_2 (80 wt% enriched uranium). We used the nu*fission cross sections of the detector as the source for the adjoint equation. These regions are homogenized in y-direction. The fine mesh size of 0.25 cm x 0.25 cm x 0.25 cm was used in both PARTISN and MUST code calculations. In the calculation with MUST code, each fine mesh was further divided into six tetrahedral meshes.

At first, the forward transport calculations were performed by MUST and PARTISN code to determine the forward scalar flux in the detector region. The results are compared in Fig. 2 where the maximum difference between MUST and PARITSN is 2.8 %.

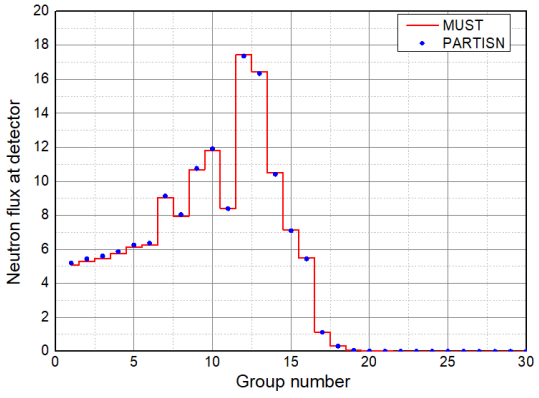

Fig. 2. Comparison of forward scalar fluxes in detector region

Next, we estimated the detector response which is calculated by

$$R=\int dV\int dE\,\nu\sigma_f(r_d,E)\phi(r_d,E) \quad (7)$$

where $\phi(r_d, E)$ represents the forward scalar flux at energy E in the detector region. This detector response can be also calculated using the adjoint scalar flux as follows:

$$R = \int dV \int dE\, \phi^+(r,E) q_{ex}(r,E) \qquad (8)$$

Table I compares the detector responses calculated with the forward and adjoint scalar fluxes obtained using MUST and PARITSN. As shown in Table I, the detector responses calculated with the forward and adjoint scalar fluxes for each code are exactly same, which verifies the adjoint solutions, and the discrepancy in the detector response between two codes is about 1.07%.

Table I: Comparison of the detector responses

Flux type	MUST	PARTISN	Discrepancy (%)
Forward	63.53	64.22	1.07
Adjoint	63.53	64.23	1.07

The results of the adjoint scalar flux in the source region are compared in Fig. 3 where the maximum different between MUST and PARTISN code is 3.2 %.

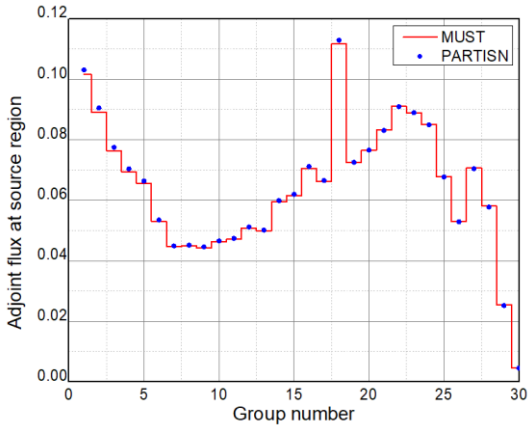

Fig. 3. Comparison of adjoint scalar fluxes in the source region

4.2. Eigenvalue problem

In this sub-section, a homogeneous eigenvalue problem composed of ^{235}U is considered to validate the MUST adjoint calculation. We assumed that the atomic density of ^{235}U in the medium is 2.713×10^{-2} atom/barn.cm. The problem domain is 9 cm x 1 cm x 1 cm in x, y and z-directions, respectively. The problem domain was divided into 9 coarse meshes for x-direction and so each coarse mesh is a 1 cm x 1 cm x 1 cm cube. Each coarse mesh was further divided into 64 fine meshes. In the calculation with MUST code, each fine mesh is divided into six tetrahedral meshes of equal volume. In this problem, we assumed the reflective boundary conditions in y- and z-directions, and the vacuum boundary conditions were applied in x-direction. The forward and adjoint transport calculations were performed by the MUST and PARTISN codes to determine the effective neutron multiplication factor (k_{eff}). The k_{eff} values obtained from MUST and PARTISN calculations are given in Table II which show that the discrepancy in k_{eff} is just 46.1 pcm and that the forward and adjoint calculations give exactly the same results. The normalized forward scalar fluxes in the center coarse mesh are compared in Fig. 4, where the maximum discrepancy between two codes is less than 0.2 %.

Table II: Comparison of k_{eff} values

Calculation type	MUST	PARTISN	Discrepancy (pcm)
Forward	0.84617	0.84584	46.1
Adjoint	0.84617	0.84584	46.1

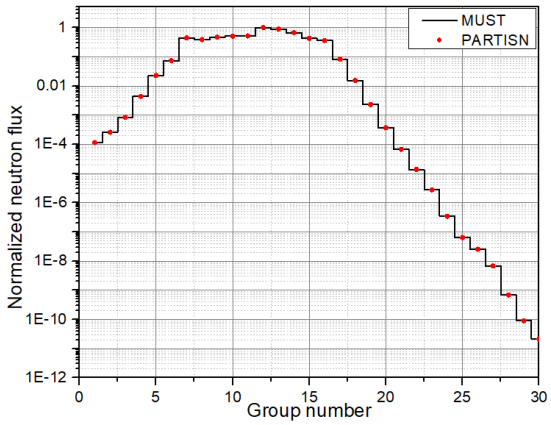

Fig. 4. Comparison of the normalized forward scalar fluxes in center coarse mesh

The adjoint flux distribution in the center coarse mesh obtained by MUST and PARTISN are compared in Fig. 5, where the maximum difference between two codes in flux distribution is less than 0.1 %.

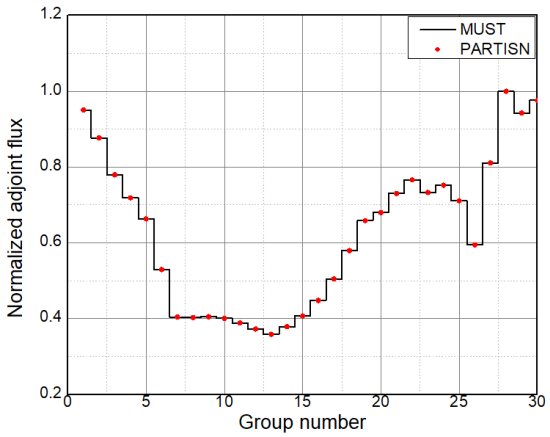

Fig. 5. Comparison of the normalized adjoint scalar fluxes in center coarse mesh

5. Conclusions

In this work, we presented the verification of the implemented adjoint transport calculation in the MUST code. The adjoint transport calculation in MUST code was aimed to use the same sweeping order as in the forward transport calculation with only modification in the source term of the transport equation. Also, we presented how the adjoint calculation can be performed using the same forward transport calculation procedure by comparing the adjoint and forward transport formulations.

In particular, the adjoint calculations in MUST code were verified with a fixed source problem and an eigenvalue problem. In the fixed source problem, the verification was performed by comparing the detector responses calculated with the forward flux in the detector and the adjoint flux in the neutron source, and by directly comparing the forward and adjoint scalar fluxes obtained with MUST and PARTISN. In the eigenvalue problem, the adjoint transport calculation of MUST was verified by showing that the adjoint and forward calculations give exactly the same eigenvalues and by comparing the eigenvalues and forward and adjoint scalar fluxes obtained with MUST and PARTISN. From the verifications, it is concluded that the adjoint calculation is successfully implemented in MUST.

Acknowledgments

This work was supported by the NRF (National Research Foundation of Korea) through Project No. NRF-2019M2D2A1A02057890.

REFERENCES

[1]. G.I. Bell, S. Glasstone, “Nuclear Reactor Theory”, 1970.
[2]. S.G. Hong, J.W. Kim, and Y. Lee, “Development of MUST (Multi-group Unstructured geometry S_N Transport) Code”, Transaction of the Korean Nuclear Society Autumn Meeting, Gyeongju, Korea, 2009.
[3]. S.G. Hong, “Two Subcell Balance Methods for Solving the Multigroup Discrete Ordinates Transport Equation with Tetrahedral Meshes”, Nuclear Science and Engineering, 173, 101-107, 2013.
[4]. R. E. Alcouffe, R. S. Baker, J. A. Dahl, S.A. Turner, and R.C. Ward, “PARTISN: A Time-Dependent, Parallel Neutral Particle Transport Code System” manual, LA-UR-05-3925, LANL, 2005.