MUST Code Solutions for the Two Group Eigenvalue Problems

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

In the reactor physics calculation, solutions for the neutron transport equation are obtained mostly by the discrete ordinates method, referred as an S_N method. A number of computer codes that use S_N method require regular mesh (such as rectangular, cylindrical or spherical) to model the problems 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.

In the reactor physics problem, it is difficult to represent cylindrical fuel pellet, gap, and cladding with regular meshes. This is why we use pin cell homogenized cross sections.

The MUST (**M**ulti-group **U**nstructured geometry $\mathbf{S}_N$ **T**ransport) code [1] uses unstructured tetrahedral elements so that it can solve pin cell or fuel assembly without using the homogenized cross sections.

In this paper, the k_{eff} calculation results of MUST code are compared with that of MCNP5 [2] reference calculation.

2. Method and results

2.1 Brief Introduction of the Theory and Method that MUST Code Uses

The starting equation is the neutral particle transport equation as

$$\vec{\Omega}_m \bullet \nabla \varphi_{m,g}(\vec{r}) + \sigma_{t,g}(\vec{r})\varphi_{m,g}(\vec{r}) = S_{m,g}(\vec{r}) + Q_{m,g}(\vec{r}), \quad (1)$$

where *m* and *g* are the ordinate and the energy group indexes respectively.

In DFEM (Discontinuous Finite Element Method), the problem domain is divided into tetrahedral elements. In each element, the flux is expanded in terms of the trial functions as follows:

$$\varphi_{m,g}(\vec{r}) = \vec{\Theta}^T(\vec{r})\vec{\psi}_{m,g} = \sum_{p=1}^{P} \psi_{m,g,p}\gamma_p(\vec{r}), \quad (2)$$

where $\gamma_p(\vec{r})$ are the trial functions and P is the number of the trial functions. The trial function $\gamma_p(\vec{r})$ should be unity at $\vec{r}_p$ but it should be zero at the other node points.

We integrate Eq. (1) over a tetrahedral element (k) after substituting Eq. (2) into Eq. (1), then we have

$$\sum_{l=1}^{N_f} \int_{A_{k,l}} \hat{\Omega}_m \cdot \hat{n}_{k,l} \vec{\Theta}\vec{\Theta}^T \vec{\psi}^{s,k,l}_{m,g} dA - \hat{\Omega}_m \cdot \int_{V_k} [\nabla\vec{\Theta}]\vec{\Theta}^T \vec{\psi}_{k,m,g} dV \quad (3)$$
$$+ \int_{V_k} \sigma_g \vec{\Theta}\vec{\Theta}^T \vec{\psi}_{k,m,g} dV = \int_{V_k} \vec{\Theta}\vec{\Theta}^T [\vec{s}_{k,m,g} + \vec{q}_{k,m,g}] dV.$$

Rewrite Eq. (3) as a matrix and vector form and the incoming faces are separated from the outgoing faces,

$$[\sum_{l=1}^{N_{f\_out}} U^{out}_{m,k,l} + K_{m,k} + \sigma_g M_k]\vec{\psi}_{k,m,g} = M_k(\vec{s}_{k,m,g} + \vec{q}_{k,m,g}) \quad (4)$$
$$+ \sum_{l=1}^{N_{f\_in}} U^{in}_{m,k,l} \vec{\psi}_{\alpha\{l\},m,g},$$

where

$$[K_{m,k}]_{ij} = -\int_{V_k} [\mu_m \frac{\partial \gamma_i}{\partial x} + \eta_m \frac{\partial \gamma_i}{\partial y} + \xi_m \frac{\partial \gamma_i}{\partial z}]\gamma_j dV,$$
$$[M_k]_{ij} = \int_{V_k} \gamma_i \gamma_j dV, \quad (5)$$
$$[U_{m,k,l}]_{ij} = \int_{A_{k,l}} |\hat{\Omega}_m \cdot \hat{n}_{k,l}| \gamma_i \gamma_j dA.$$

The integration and differentiations in Eq. (5) are performed in a local barycentric coordinate in order to simplify the calculations. The calculated results are transformed into the ones of global coordinates. This transformation needs the volumetric and surface Jacobians.

2.2 Test and Results

For the eigenvalue benchmark calculations, we devise two test problems. One is simple nested cube problem and the other is 6x6 fuel assembly without homogenization. The unstructured tetrahedral elements are generated by GMSH [3] and Tetgen [4] codes. The reference k_{eff}s are calculated by MCNP5 with the identical two group cross section data.

The configuration of the Test Problem I is shown in the Fig. 1. The cross section for the fuel and moderator are listed in the Table I.

The total number of tetrahedral element is 8551 and calculations are performed with varying S_N quadrature.

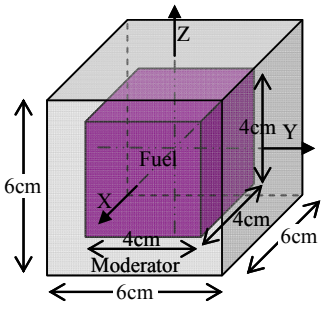

Fig. 1. The configuration of the Test Problem I.

With the Test Problem II, we like to show how MUST code represents fuel, cladding, and guide thimble without homogenization. Most three dimensional discrete ordinates code that use regular mesh (i.e., rectangular) has some difficulties to represent this complicate geometry.

The configuration of the Test Problem II is shown in Fig. 2 and the cut view of unstructured tetrahedral elements is shown in the Fig. 3. In the fuel rod modeling, gap is neglected. The inner and outer radius of the fuel rod are 0.4215cm and 0.4850cm respectively. For the guide tube, inner and outer radius are 1.1430cm and 1.2446cm respectively. In the geometry modeling, 277850 tetrahedral elements are used.

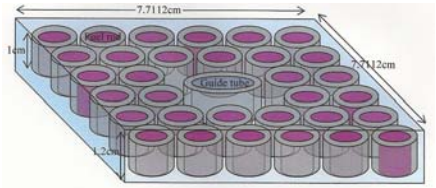

Fig. 2. The configuration of the Test Problem II.

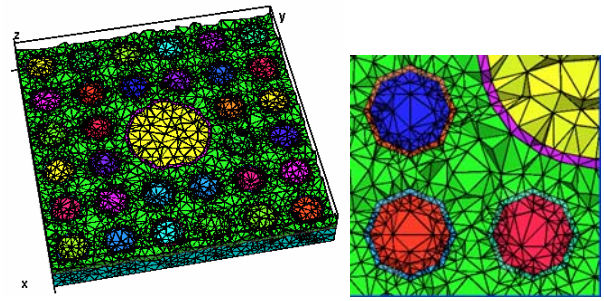

Fig. 3. The cut view of unstructured tetrahedral elements.

The macroscopic cross sections for each region are listed in Table I. The calculations are performed with varying S_N quadrature.

Table I: Cross sections

	Fuel (cm^{-1})	Moderator (cm^{-1})	Cladding (cm^{-1})
$\sigma_{tot,1}$	1.09295e+1	1.57862e+0	2.77940e-1
$\nu\sigma_{f,1}$	2.05744e+1	-	-
$\sigma_{s,1\rightarrow1}$	6.94948e-1	6.41100e-1	2.44230e-1
$\sigma_{s,1\rightarrow2}$	6.08324e-3	9.30400e-1	2.90088e-2
$\sigma_{tot,2}$	1.34828e+2	6.42604e+0	2.95630e-1
$\nu\sigma_{f,2}$	2.74896e+2	-	-
$\sigma_{s,2\rightarrow1}$	-	-	-
$\sigma_{s,2\rightarrow2}$	7.81572e-1	6.34300e+0	2.870538e-1

The k_{eff} results for the two test problems are listed in the Table II. The difference of k_{eff} for the Test Problem I is about a few pcm. However, that of the Test Problem II is about a few hundred pcm. In the Test Problem II, we could not perform the calculation with higher quadrature due to the memory problem.

Table II: The k_{eff} results

	Test Problem I		Test Problem II	
Reference (MCNP5)	2.00179±0.00001		1.87411±0.00001	
S_N order	k_{eff}	Difference Δρ (pcm) †	k_{eff}	Difference Δρ (pcm)
2	2.00163	-4	1.84755	-767
4	2.00168	-3	1.86048	-391
6	2.00169	-3	1.86284	-323
8	2.00169	-2	N/A	
10	2.00169	-2		
12	2.00169	-2		
14	2.00169	-2		
16	2.00169	-2		
18	2.00169	-2		
20	2.00169	-2		

†Difference Δρ (pcm) = $[(k_{eff}-k_{eff,\,Reference})/(k_{eff}\times k_{eff,\,Reference})]\times10^5$

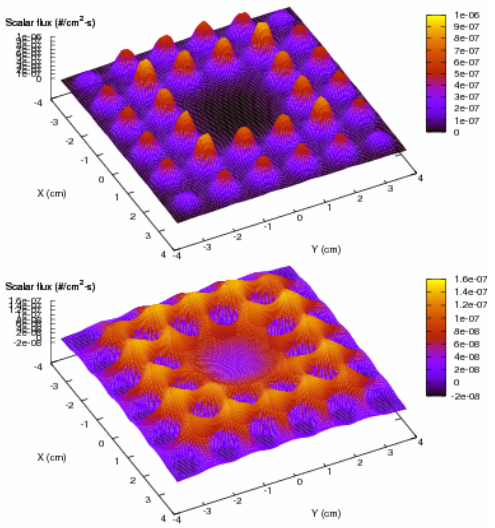

Fig. 4. The scalar flux of the 1st and 2nd group (Test Problem II, at z=0.5).

3. Conclusions

The k_{eff} results of two test problems are presented and compared with the reference MCNP5 calculations.

The numerical tests show that unstructured tetrahedral elements are flexible to model complicate geometry (e.g., 6x6 fuel assembly). However, compared to the reference calculation, there are still big differences.

For better results, S_N code like MUST should use more elements to model the arc of cylinder accurately. However, this may cause the memory problems that we should break through.

Acknowledgement

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