New Three-Dimensional Neutron Transport Calculation Capability in STREAM Code

Youqi Zheng [a,b], Sooyoung Choi [b], Deokjung Lee [b*]
[a] *Xi'an Jiaotong University, No. 28, Xianning West Road, Xi'an, Shaanxi 710049, China*
[b] *Ulsan National Institute of Science and Technology, UNIST-gil 50, Ulsan 689-798, Republic of Korea*
[*] *Corresponding author: deokjung@unist.ac.kr*

1. Introduction

The 3D neutron transport calculation with pin or sub-pin resolutions is becoming more and more attractive in current reactor simulations. The method of characteristics (MOC) is one of the best choices for its powerful capability in the geometry modeling. To reduce the large computational burden in 3D MOC, the 2D/1D schemes were proposed and have achieved great success in the past 10 years [1-3]. However, such methods have some instability problems during the iterations when the neutron leakage for axial direction is large. Therefore, full 3D MOC methods were developed. A lot of efforts have been devoted to reduce the computational costs [4, 5]. However, it still requires too much memory storage and computational time for the practical modeling of a commercial size reactor core.

Recently, a new approach for the 3D MOC calculation without transverse integration has been implemented in the STREAM code. In this approach, the angular flux is expressed as a basis function expansion form of only axial variable *z* [6]. Then, the 3D neutron transport equation is transformed into the 2D form of the expansion coefficients. The MOC sweeping is used to get the coefficients with multi-group CMFD acceleration. Numerical tests based on the 3D KUCA and C5G7 benchmarks are performed to verify the new capability of STREAM code.

2. Methods

The multi-group three-dimensional neutron transport equation is expressed as:

$$\mu_n \frac{\partial \psi_{g,n}(\vec{r})}{\partial x} + \eta_n \frac{\partial \psi_{g,n}(\vec{r})}{\partial y} + \xi_n \frac{\partial \psi_{g,n}(\vec{r})}{\partial z} + \Sigma_{tg} \psi_{g,n}(\vec{r}) = q_{g,n,s}(\vec{r}) + q_{g,n,f}(\vec{r}) \quad (1)$$

where, $q_{g,s}$ and $q_{g,f}$ are the fission source and scattering source as:

$$q_{g,n,s}(\vec{r}) = \frac{1}{4\pi} \sum_{g'=1}^{G} \int \Sigma_{g'g}(\vec{r}, \Omega' - \Omega) \psi_{g'}(\vec{r}, \Omega') d\Omega'$$

$$q_{g,n,f}(\vec{r}) = \frac{\chi_g}{4\pi k_{eff}} \sum_{g'=1}^{G} \int \Sigma_{fg'}(\vec{r}) \psi_{g'}(\vec{r}, \Omega') d\Omega'$$

2.1 Axial Linear Expansion model

Supposing the radial and axial dependence of angular flux can be separately treated and the axial dependence can be expanded by a linear basis function as:

$$\psi_n(\vec{r}) = \sum_{m=1}^{2} \psi_{m,n}(x,y) b_m(z), \quad (2)$$

where $b_1(z) = 1$ and $b_2(z) = \frac{2}{\Delta z}\left(z - \bar{z}\right)$.

Submitting the flux expansion into the transport equation (1), and using the discontinuous finite element method in the axial direction, the 3D equation is transformed into a set of 2D equations for every axial plane *p* as:

$$\begin{aligned} &\mu_n \frac{\partial \psi^p_{1,n}(x,y)}{dx} + \eta_n \frac{\partial \psi^p_{1,n}(x,y)}{dy} + \left(\Sigma^p_t + \frac{\xi_n}{\Delta z}\right)\psi^p_{1,n}(x,y) \\ &\quad = Q^p_{1,n}(x,y) + \frac{\xi_n}{\Delta z}\psi^{p,-}_n(x,y) - \frac{\xi_n}{\Delta z}\psi^p_{2,n}(x,y), \\ &\mu_n \frac{\partial \psi^p_{2,n}(x,y)}{dx} + \eta_n \frac{\partial \psi^p_{2,n}(x,y)}{dy} + \left(\Sigma^p_t + \frac{3\xi_n}{\Delta z}\right)\psi^p_{2,n}(x,y) \\ &\quad = Q^p_{2,n}(x,y) - \frac{3\xi_n}{\Delta z}\psi^{p,-}_n(x,y) + \frac{3\xi_n}{\Delta z}\psi^p_{1,n}(x,y), \end{aligned} \quad \xi_n > 0 \quad (3)$$

and

$$\begin{aligned} &\mu_n \frac{\partial \psi^p_{1,n}(x,y)}{dx} + \eta_n \frac{\partial \psi^p_{1,n}(x,y)}{dy} + \left(\Sigma^p_t - \frac{\xi_n}{\Delta z}\right)\psi^p_{1,n}(x,y) \\ &\quad = Q^p_{1,n}(x,y) - \frac{\xi_n}{\Delta z}\psi^{p,+}_n(x,y) - \frac{\xi_n}{\Delta z}\psi^p_{2,n}(x,y), \\ &\mu_n \frac{\partial \psi^p_{2,n}(x,y)}{dx} + \eta_n \frac{\partial \psi^p_{2,n}(x,y)}{dy} + \left(\Sigma^p_t - \frac{3\xi_n}{\Delta z}\right)\psi^p_{2,n}(x,y) \\ &\quad = Q^p_{2,n}(x,y) - \frac{3\xi_n}{\Delta z}\psi^{p,+}_n(x,y) + \frac{3\xi_n}{\Delta z}\psi^p_{1,n}(x,y), \end{aligned} \quad \xi_n < 0 \quad (4)$$

where

$$\psi^+_n = \psi_{1,n}(x,y) + \psi_{2,n}(x,y), \quad (5)$$

$$\psi^-_n = \psi_{1,n}(x,y) - \psi_{2,n}(x,y). \quad (6)$$

Equation (3) and (4) can be solved by using the traditional MOC sweeping as:

$$\begin{aligned} &\cos\theta_j \frac{d\psi^p_{1,n}(x,y)}{ds} + \left(\Sigma^p_t + \frac{\xi_n}{\Delta z}\right)\psi^p_{1,n}(x,y) = S^p_{1,n}(x,y), \\ &\cos\theta_j \frac{d\psi^p_{2,n}(x,y)}{ds} + \left(\Sigma^p_t + \frac{3\xi_n}{\Delta z}\right)\psi^p_{2,n}(x,y) = S^p_{2,n}(x,y), \end{aligned} \quad \xi_n > 0 \quad (7)$$

and

$$\begin{aligned}\cos\theta_j \frac{d\psi^p_{1,n}(x,y)}{ds} + \left(\Sigma^p_t - \frac{\xi_n}{\Delta z}\right)\psi^p_{1,n}(x,y) = S^p_{1,n}(x,y), \\ \cos\theta_j \frac{d\psi^p_{2,n}(x,y)}{ds} + \left(\Sigma^p_t - \frac{3\xi_n}{\Delta z}\right)\psi^p_{2,n}(x,y) = S^p_{2,n}(x,y).\end{aligned} \quad \xi_n < 0 \tag{8}$$

The boundary conditions and interface conditions are used to couple all the axial planes together. In the current work, the vacuum and reflective boundary conditions are considered. The angular flux continuity is adopted as the interface condition.

2.2 CMFD Acceleration

The multi-group CMFD equation in the three-dimensional coarse mesh *m* is expressed as:

$$\begin{aligned}&\sum_{u=x,y,z}\frac{1}{h^u_m}\left[J^{m,+}_{gu} - J^{m,-}_{gu}\right] + \Sigma^m_{tg}\phi^m_g \\ &= \frac{\chi_g}{k_{eff}}\sum_{g'=1}^{G}\nu\Sigma^m_{fg'}\phi^m_{g'} + \sum_{g'=1}^{G}\Sigma^m_{g'g}\phi^m_{g'}\end{aligned} \tag{9}$$

and

$$J^{m,\pm}_{gu} = \mp D^{m\pm}_{gu}\left(\phi^{m\pm1_u}_g - \phi^m_g\right) - D^{m\pm}_{gu}\left(\phi^{m\pm1_u}_g + \phi^m_g\right), \tag{10}$$

where $J^{m,\pm}_{gu}$ is the surface net current of coarse mesh *m* in *u* direction, + stands for the right surface and – is the left one. It is obtained by the higher order MOC calculation as:

$$J^{\pm}_{g,x} = \frac{1}{\Delta y}\sum_n \omega_n \cos\theta_j \cos\varphi_i \sum_k \psi^{x^\pm}_{g,1,n,k}\Delta y_k \ , \tag{11}$$

$$J^{\pm}_{g,y} = \frac{1}{\Delta x}\sum_n \omega_n \cos\theta_j \sin\varphi_i \sum_k \psi^{y^\pm}_{g,1,n,k}\Delta x_k \ , \tag{12}$$

$$J^{\pm}_{g,z} = \sum_n \omega_n \sin\theta_j \psi^{\pm}_{g,n,fsr} \ , \tag{13}$$

where *k* is the index of MOC tracks. Then, the corrected diffusion coefficient is updated as:

$$D^{m\pm}_{gu} = \frac{\mp D^{m\pm}_{gu}\left(\phi^{m\pm1_u}_g - \phi^m_g\right)}{\left(\phi^{m\pm1_u}_g + \phi^m_g\right)} - \frac{J^{m,\pm}_{gu}}{\left(\phi^{m\pm1_u}_g + \phi^m_g\right)}. \tag{14}$$

The fission source and scattering source in the high order transport equation (1) are updated based on the new scalar flux obtained from solving Eq. (9).

3. Numerical Tests

The STREAM code is updated to be capable of solving the 3D multi-group neutron transport equation. In this paper, two benchmark problems are calculated to verify the new capability.

First, the KUCA benchmark problem is calculated. This problem is simplified from the Kyoto University Critical Assembly (KUCA). It models a 1/8 core of a thermal reactor with reflective boundary conditions. There are three regions: core, control rod, and reflector. The size is 25cm × 25cm × 25cm. The detailed specification can be found in the literature [7].

The results of Keff for rodded and unrodded cases are shown in table I. In the STREAM calculation, the sub-mesh with size of 1cm × 1cm × 1cm is divided. Six polar angles and 48 azimuthal angles are used. Around 200 MB memory is allocated for the quadrature.

Two reference results are compared by using the multi-group Monte-Carlo code and P_N code (VARIANT). The Keff results show good agreements with the two codes.

Table I: Keff Results of KUCA Benchmark

	Keff		Rod worth
	Rod_out	Rod_in	
Reference/MC	0.97800 (0.0006[a])	0.96240 (0.0006)	1.66e-02 (0.09e-02)
Reference/P_N	0.97660 (-0.14[b])	0.96300 (0.06)	1.45e-02 (-12.7)
STREAM	0.97669 (-0.13)	0.96173 (-0.07)	1.59e-02 (-4.2)

a: standard deviation
b: relative error in percent

Then, the C5G7 benchmark is calculated. This benchmark has been widely used to verify the 3D neutron transport solver with pin resolution. It consists of 3 cases including one unrodded case and two rodded cases. The detailed specification can be referred from the benchmark report [8].

Tables II-IV summarize the results of 3 cases. In the STREAM calculation, 45 axial planes are divided. In the 2D MOC sweeping, 64 flat source regions are divided for each pin cell. Eight polar angles and 32 azimuthal angles are used. The reference results are all from the multi-group Monte-Carlo calculations given in the benchmark report.

Table II: Keff Results of C5G7 Benchmark

	Unrodded	Rodded A	Rodded B
Reference	1.14308	1.12806	1.07777
STREAM	1.14222	1.12729	1.07685
Error(pcm)	-66	-61	-79

Table III: Max. Pin Power Results of C5G7 Benchmark

	Unrodded	Rodded A	Rodded B
Reference	2.481	2.253	1.834
STREAM	2.474	2.245	1.830
Error(%)	-0.29	-0.36	-0.25

Table IV: Summarization of other Parameters

	Unrodded	Rodded A	Rodded B
AVG(%)	0.30	0.29	0.28
RMS(%)	0.41	0.38	0.38
MRE(%)	0.23	0.23	0.24
Memory cost (GB)	4.7	4.7	4.7
CPU time (hour)	27	29	27

The results prove good accuracy of STREAM in the 3D transport calculations for both Keff and pin power prediction. The memory cost is not a big problem even parts of the angular flux should be stored for the plane-wise coupling in the axial direction. The computational time is still very long even with CMFD acceleration due to the fine axial mesh. In current STREAM, the linear basis function is applied in the *z* direction, the axial meshes as small as 1-2cm are necessary for the heterogeneous problems, which requires a lot of MOC sweeping.

4. Conclusions

A new approach based on the axial expansion and 2D MOC sweeping to solve the 3D neutron transport equation is implemented in the STREAM code. This approach avoids using the transverse integration in the traditional 2D/1D scheme of MOC calculation. By converting the 3D equation into the 2D form of angular flux expansion coefficients, it also avoids the complex 3D ray tracing. Current numerical tests using two benchmarks show good accuracy of the new method. More tests will be done in the next work for a real PWR fuel assembly or core problems.

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