A Study on Consistency of Nodal Methods Using Transverse Leakage Approximation

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1. Introduction

Since the development of the transverse-integrated Nodal Expansion Method (NEM) in the 1970s [1], it has been widely utilized in modern multi-dimensional whole-core neutronic simulations due to its relatively low computational cost and high accuracy compared to traditional finite-difference methods.

In NEM, the transverse leakage (TL) approximation is a critical concept for handling the leakage term via current along the surface. Under the assumption that flux shapes are not highly sensitive to the TL shape, a quadratic polynomial is typically adopted to represent the TL term. This approach has been proven to perform well for typical Light Water Reactor (LWR) problems.

One of the most popular methods to determine the coefficients for the TL term involves assuming linearity over three adjacent nodes in a given direction, applying interface conditions. However, it has been observed that the aforementioned method can lead to inconsistencies in eigenvalue problems when applied within the Source Expansion Nodal Method (SENM) framework in this study. In the contrast, an alternative TL approximation that conserves the node-average TL values across three adjacent nodes in a direction has shown more reasonable results in both k_{eff} and power distribution for certain problems without sacrificing its consistency.

In this paper, the implementation of these approximations within the multi-physics Pressurized Water Reactor (PWR) core simulator KANT [2] will be discussed with detailed mathematical expressions. Additionally, a comparison of k_{eff} and power distribution results will be presented and analyzed.

2. Methods

2.1 TL approximation with assuming linearity [3]

In most modern nodal methods, the quadratic polynomial is a common choice for representing the TL shape. The only given values are the node-averaged TLs, calculated from line-averaged surface neutron currents, and the other unknown coefficients related to the quadratic polynomial must be determined with appropriate assumptions. The mathematical expression for the quadratic polynomial in the l-th node in Fig. 1 can be written as follows:

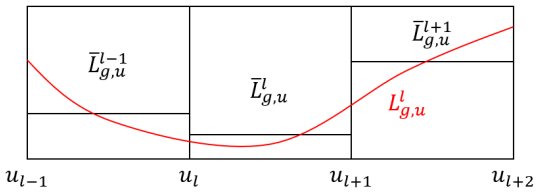

Figure 1. Transverse leakage with adjacent three nodes

$$L_{g,u}^{l}(u) \approx tl_{g,u,0}^{l} P_0\left(\frac{u-u_l}{h_u^l}\right) + tl_{g,u,1} P_1\left(\frac{u-u_l}{h_u^l}\right) + tl_{g,u,2} P_2\left(\frac{u-u_l}{h_u^l}\right), \quad u \in [u_l, u_{l+1}] \tag{1}$$

where u is a direction in the transverse-integrated 1D diffusion equation, g is a g-th energy group, h_u^l is the size of the l-th node in u-direction, and $P_n(u)$ is the n-th order basis function used in NEM or SENM kernel.

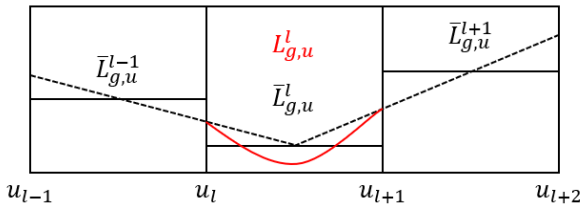

Figure 2. Transverse leakage term in the l-th node with assuming linearity.

In this approximation, three unknown coefficients, $tl_{g,u,0}^{l}$, $tl_{g,u,1}^{l}$, $tl_{g,u,2}^{l}$ are determined by assuming linearity, which means that the gradient at the interface can be represented linearly. With this approach, we assume that at the interface between two adjacent nodes, the gradient values, when multiplied by each node's diffusion coefficient D_g^l, should be equal, as should the TL values of the two nodes at the interface as shown in Fig. 2.

$$L_{g,u}^{l-1}(u_l) = L_{g,u}^{l}(u_l) \tag{2}$$

$$D_g^{l-1} \left.\frac{dL_{g,u}^{l-1}(u)}{du}\right|_{u=u_l} = D_g^{l} \left.\frac{dL_{g,u}^{l}(u)}{du}\right|_{u=u_l} \tag{3}$$

And if we define the $L^l_{g,u}$ values at the left and right interface of the l-th node as $L^l_{g,u,l}$ and $L^l_{g,u,r}$ respectively, they can be rewritten as follows by assuming linearity:

$$L^l_{g,u,l} \equiv \frac{\frac{D^{l-1}_g}{h^{l-1}_u}\bar{L}^{l-1}_{g,u} + \frac{D^l_g}{h^l_u}\bar{L}^l_{g,u}}{\frac{D^{l-1}_g}{h^{l-1}_u} + \frac{D^l_g}{h^l_u}} = L^l_{g,u}(u_l) \quad (4)$$

$$L^l_{g,u,r} \equiv \frac{\frac{D^l_g}{h^l_u}\bar{L}^l_{g,u} + \frac{D^{l+1}_g}{h^{l+1}_u}\bar{L}^{l+1}_{g,u}}{\frac{D^l_g}{h^l_u} + \frac{D^{l+1}_g}{h^{l+1}_u}} = L^l_{g,u}(u_{l+1}) \quad (5)$$

Additionally, if a reflective boundary condition is imposed on the left boundary of the l-th node at $u = u_l$, $L^l_{g,u}(u_l)$ becomes $\bar{L}^l_{g,u}$. Conversely, if a vacuum boundary condition is imposed on the right boundary of the l-th node at $u = u_{l+1}$, $L^l_{g,u}(u_{l+1})$ becomes 0. Consequently, the all coefficients for the TL quadratic polynomial can be determined.

2.2 TL approximation conserving 3 adjacent average TLs [3]

This approximation shares the same mathematical expression - second-order polynomial - for TL, and the only given values are node-averaged TLs of each three nodes as in the case of aforementioned TL approximation. However, there are significant differences in the procedure for determining three unknown coefficients, $tl^l_{g,u,0}, tl^l_{g,u,1}, tl^l_{g,u,2}$ of the Eq. (1). In the previous approximation, we only focused on the TL distribution of the l-th node, using the adjacent node-averaged TL values to determine unknown coefficients for the l-th node. In this approximation, the TL distributions of each adjacent three nodes are subject to be determined together, and the node-averaged TL values should be conserved.

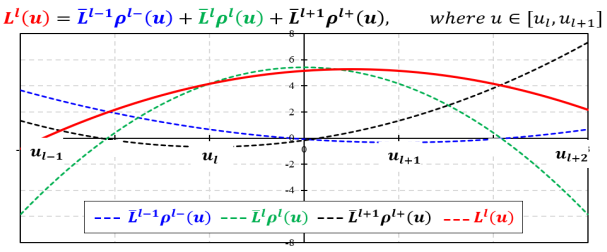

Figure 3. Transverse leakage term in the l-th node conserving 3 adjacent average TLs.

The key idea of this approximation is that the TL distribution of the l-th node is a combination of three adjacent nodes, including the l-th node and they affect adjacent nodes simultaneously as shown in Fig 3.

The TL distribution of the l-th node is defined as follows:

$$L^l_{g,u}(u) \approx \bar{L}^{l-1}_{g,u}\rho^{l-1}_u\left(\frac{u-u_l}{h^l_u}\right) + \bar{L}^l_{g,u}\rho^l_u\left(\frac{u-u_l}{h^l_u}\right) + \bar{L}^{l+1}_{g,u}\rho^{l+1}_u\left(\frac{u-u_l}{h^l_u}\right), \quad (6)$$

where $u \in [u_l, u_{l+1}]$,

$$\rho^{l-1}_u(u) = a^{l-}_u P_0\left(\frac{u-u_l}{h^l_u}\right) + b^{l-}_u P_1\left(\frac{u-u_l}{h^l_u}\right) + c^{l-}_u P_2\left(\frac{u-u_l}{h^l_u}\right) \quad (7)$$

$$\rho^l_u(u) = a^{l0}_u P_0\left(\frac{u-u_l}{h^l_u}\right) + b^{l0}_u P_1\left(\frac{u-u_l}{h^l_u}\right) + c^{l0}_u P_2\left(\frac{u-u_l}{h^l_u}\right) \quad (8)$$

$$\rho^{l+1}_u(u) = a^{l+}_u P_0\left(\frac{u-u_l}{h^l_u}\right) + b^{l+}_u P_1\left(\frac{u-u_l}{h^l_u}\right) + c^{l+}_u P_2\left(\frac{u-u_l}{h^l_u}\right) \quad (9)$$

and $P_n(u)$ is the n-th order basis function used in NEM or SENM kernel. Then, the 9 unknown coefficients can be determined by:

$$\frac{1}{h^{l+l'}_u}\int_{l+l'}^{u_{l+l'+1}} \rho^{l+l''}_u(u)\,du = \delta_{l'l''}, \quad (10)$$

where $\delta_{l'l''}$ is the Kronecker delta and l' = -1,0,1 and l'' = -1,0,1.

For the boundary condition, if a reflective boundary condition is imposed on the left boundary of the l-th node at $u = u_l$, $\bar{L}^{l-1}_{g,u}$ becomes $\bar{L}^l_{g,u}$. Conversely, if a vacuum boundary condition is imposed on the right boundary of the l-th node at $u = u_{l+1}$, $\bar{L}^{l+1}_{g,u}$ becomes 0.

3. Numerical Results

In order to examine the performance of two different TL approximations, these methods are implemented in the KANT code developed at KAIST [2]. The benchmark problems used in this paper consist of well-known cases. The representative two-group, two-dimensional problems IAEA2D [4] and BIBLIS2D [4] were tested, as well as the multi-group problem KOEBERG 4G [4]. To evaluate the validity of two TL approximations in a situation where a sudden change in the gradient of neutron flux is expected, the L336C5 [5] benchmark, which originally involves pin-wise heterogeneous configuration, was analyzed using the NEM and SENM kernels. The assembly-homogenized cross sections were generated through flux-volume-weighted method with fine mesh FDM, where the mesh size is 0.008568 cm. Additionally, the IAEA3D [6] problem, where control rods are partially inserted at the assembly level, was also tested. Both the error tolerance

of k_{eff} and fission source distribution were set to 10^{-8}, and the conventional two-node coarse-mesh finite difference (CMFD) method was utilized for acceleration and invoked every 20 outer cycles. In terms of notation for TL approximations, the one assuming linearity is denoted as TL1, and the other one conserving the average TL values of three adjacent nodes is denoted as TL2 for convenience. Therefore, there are four types of calculations: NEN-TL1, NEM-TL2, SENM-TL1, and SENM-TL2, which are referred to as N1, N2, S1, and S2, respectively, in this paper.

The reference solution for k_{eff} of the L336C5 problem is 0.938132, and calculations were conducted for all types under three different node size conditions.

Table 1. k_{eff} error and assembly power error variation with node size of L336C5 problem

Type	1x1		2x2		4x4	
	k_{eff} (pcm)	power (%)	k_{eff} (pcm)	power (%)	k_{eff} (pcm)	power (%)
N1	-274	2.01	-44	0.33	1	0.06
N2	-261	2.02	-48	0.36	0	0.05
S1	4	0.43	12	0.19	5	0.07
S2	15	0.29	8	0.11	3	0.05

SENM demonstrates better accuracy than NEM in both k_{eff} and power error distribution when a steep neutron flux gradient is expected [7], such as in the presence of MOX fuel in the L336C5 case. As shown in the calculation results in the Table 1., this trend is clearly observed. In the case of S1, while the power error distribution remains consistent, the eigenvalue error is lowest for the 1x1 calculation but shows an increase in the 2x2 calculation, indicating a loss of consistency. Considering that the k_{eff} is a kind of integral value, this suggests that the agreement of the S1 type's 1x1 calculation with the reference value may be coincidental.

Table 2. Eigenvalue error and assembly power error variation with node size of other problems

Problem (Ref. k_{eff})	Type	1x1		2x2	
		k_{eff} (pcm)	power (%)	k_{eff} (pcm)	power (%)
IAEA2D (1.029585)	N1	-7	0.99	3	0.23
	N2	-2	0.23	2	0.04
	S1	5	0.98	3	0.32
	S2	8	0.27	2	0.11
BIBLIS (1.025110)	N1	-6	0.40	-3	0.11
	N2	9	0.49	0	0.12
	S1	5	0.51	-1	0.07
	S2	20	0.74	1	0.07
KOEBERG (1.007954)	N1	28	0.82	2	0.06
	N2	42	1.35	5	0.12
	S1	27	0.75	2	0.09
	S2	41	1.25	4	0.10
IAEA3D (1.029097)	N1	-7	0.71	2	0.22
	N2	-2	0.95	1	0.05
	S1	3	0.88	1	0.11
	S2	7	0.20	0	0.01

In the IAEA2D and the IAEA3D problem, when the NEM and SENM kernels were used with TL2, the power distribution error was significantly reduced compared to when TL1 was used, with reductions of up to 90% as shown in Fig. 4 and Fig. 5. Additionally, the k_{eff} error was also lower in these two problems when using TL2, except for the S2 calculation, which showed a higher error than when TL1 was used.

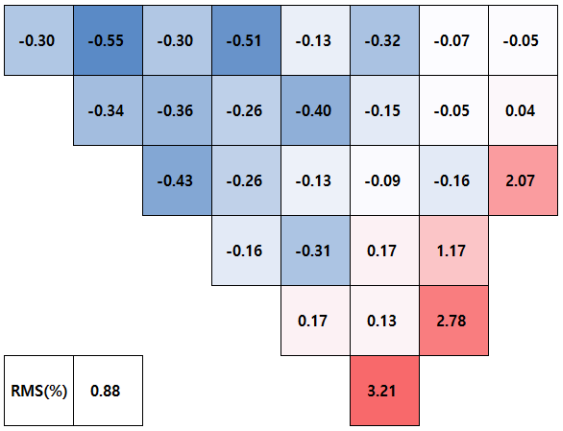

Figure 4. Assembly-wise relative power error distribution of IAEA3D problem of 1x1 S1 type

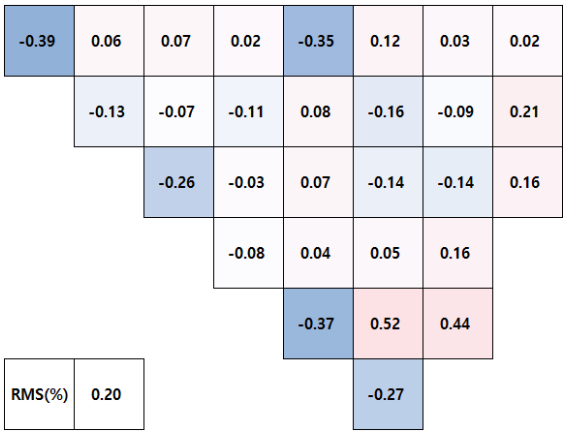

Figure 5. Assembly-wise relative power error distribution of IAEA3D problem of 1x1 S2 type

Meanwhile, in the cases of BIBLIS and KOEBERG, the TL1 option showed a tendency to be superior to TL2 in terms of k_{eff} and power error distribution. This can be interpreted as being influenced by how the TL term distribution is represented in the TL approximation and the method of approximation at the vacuum boundary.

To examine the aforementioned interpretation, the reference data of assembly-wise averaged TL distributions for the IAEA2D and BIBLIs problems were obtained using SENM calculations with 64 nodes per assembly, and are shown in Fig. 6 and Fig. 7, respectively. The power was set to 1MW_{th}.

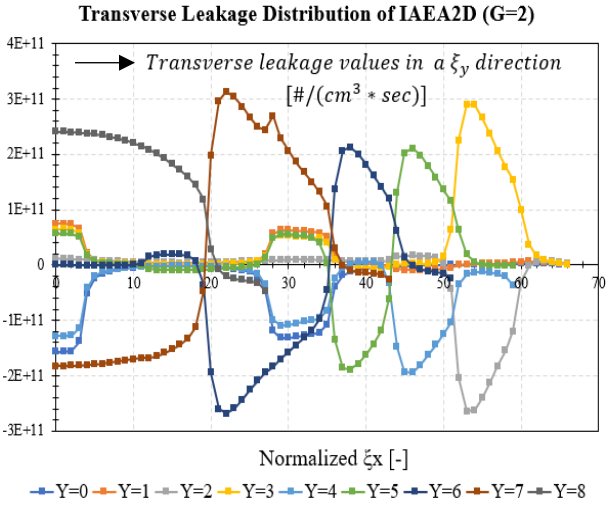

Figure 6. Reference thermal TL distribution of BIBLIS 2D problem in assembly-wise node size

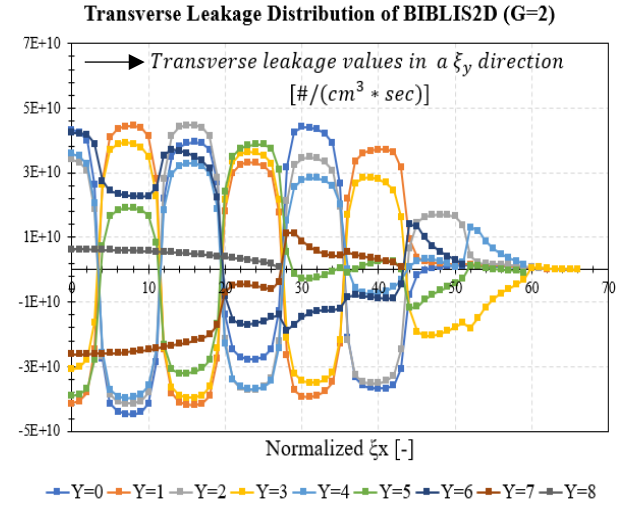

Figure 7. Reference thermal TL distribution of IAEA 2D problem in assembly-wise node size

In the case of TL1, the value of the TL term is assumed to be zero at the location where the vacuum boundary condition is applied. On the other hand, in the case of TL2, since it is expressed as the sum of a quadratic function representing the transverse leakage term for three adjacent nodes, the value is not zero at the boundary and forms curves of various shapes than TL1. If the TL term distribution in the reference solution converges nearly to zero at the vacuum boundary as shown in Fig. 6, TL1 is likely to be more accurate. However, as shown in Fig. 7, if the TL distribution in the reference solution has various form of curves and non-zero values, TL2 is likely to be more accurate.

4. Conclusions

Although it may vary depending on the problem, considering the rate of power distribution error reduction, TL2 can be an attractive option in terms of power distribution. It may offer more stable computational results than TL1 without losing its consistency. However, in cases like the BIBLIS or KOEBERG problems, where the TL assumption of a fixed zero value at the vacuum boundary is more appropriate, further research is needed to improve TL2 in terms of accuracy.

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