Solution of Mathematical Adjoint Equation for Unified Nodal Method

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1. Introduction

Recently, Lee et al [1] demonstrated that the the nodal expansion method (NEM) and the analytic nodal method (ANM), the conventional nodal methods implemented in the neutronics design and analysis codes, can be integrated into a single unified nodal method (UNM) resembles the NEM in that it makes use of the expansion of the basis functions for the solution to the transverse integrated one-dimensional (TI1D) diffusion equations. The purpose of this paper is to formulate the mathematical adjoint equation for UNM version based on the adjoint solution schemes for NEM by Kim et al [2]. This adjoint solution method is verified by comparing mathematical adjoint solution with physical adjoint solution for IAEA benchmark problems.

2. Mathematical Adjoint Equation for Unified Nodal Method

Because mathematical adjoint equations are obtained by transposing the nodal forward equations, the forward equations of UNM will be described in following section, and the adjoint equations will be derived by transposing them in the next.

2.1 Forward Equation of Unified Nodal Method

The forward equation of UNM for diffusion equations consists of the interface-current equations,

$$\begin{aligned}
\mathbf{j}_{ul}^{m-} &= 6\mathbf{Q}_{0u}^{m}\bar{\boldsymbol{\phi}}^{m} + \mathbf{Q}_{1u}^{m}\mathbf{C}_{3u}^{m} - \mathbf{Q}_{0u}^{m}\mathbf{C}_{4u}^{m} + \mathbf{Q}_{3u}^{m}\mathbf{j}_{ul}^{m+} - \mathbf{Q}_{2u}^{m}\mathbf{j}_{ur}^{m-} \\
\mathbf{j}_{ur}^{m+} &= 6\mathbf{Q}_{0u}^{m}\bar{\boldsymbol{\phi}}^{m} - \mathbf{Q}_{1u}^{m}\mathbf{C}_{3u}^{m} - \mathbf{Q}_{0u}^{m}\mathbf{C}_{4u}^{m} - \mathbf{Q}_{2u}^{m}\mathbf{j}_{ul}^{m+} + \mathbf{Q}_{3u}^{m}\mathbf{j}_{ur}^{m-}
\end{aligned} \tag{1}$$

and nodal neutron balance equation rewritten in the following form.

$$\left[\mathbf{A}^{m} + 12\sum_{u=x,y,z}\frac{1}{a_u^m}\mathbf{Q}_{0u}^{m}\right]\bar{\boldsymbol{\phi}}^{m} = \sum_{u=x,y,z}\frac{1}{a_u^m}\left[2\mathbf{Q}_{0u}^{m}\mathbf{C}_{4u}^{m} + \left(\mathbf{I} + \mathbf{Q}_{2u}^{m} - \mathbf{Q}_{3u}^{m}\right)\left(\mathbf{j}_{ul}^{m+} + \mathbf{j}_{ur}^{m-}\right)\right] \tag{2}$$

Here, all notations have the same meaning as in Ref. [1].

The $\mathbf{C}_{3u}^{m}$ and $\mathbf{C}_{4u}^{m}$ in Eq.(1), (2) are determined by the following Weight Residual Method (WRM) equations:

$$\begin{aligned}
-\mathbf{M}_{3u}^{m}\mathbf{C}_{3u}^{m} &= \mathbf{D}^{m}\left(\mathbf{B}_{3ul}^{m}\bar{\mathbf{L}}_{u}^{m-1} + \mathbf{B}_{3uc}^{m}\bar{\mathbf{L}}_{u}^{m} + \mathbf{B}_{3ur}^{m}\bar{\mathbf{L}}_{u}^{m+1}\right) \\
&\quad + \mathbf{M}_{1u}^{m}\left(\mathbf{j}_{ur}^{m+} + \mathbf{j}_{ur}^{m-} - \mathbf{j}_{ul}^{m+} - \mathbf{j}_{ul}^{m-}\right) \\
-\mathbf{M}_{4u}^{m}\mathbf{C}_{4u}^{m} &= \mathbf{D}^{m}\left(\mathbf{B}_{4ul}^{m}\bar{\mathbf{L}}_{u}^{m-1} + \mathbf{B}_{4uc}^{m}\bar{\mathbf{L}}_{u}^{m} + \mathbf{B}_{4ur}^{m}\bar{\mathbf{L}}_{u}^{m+1}\right) \\
&\quad + \mathbf{M}_{2u}^{m}\left(\mathbf{j}_{ur}^{m+} + \mathbf{j}_{ur}^{m-} + \mathbf{j}_{ul}^{m+} + \mathbf{j}_{ul}^{m-} - \bar{\boldsymbol{\phi}}^{m}\right)
\end{aligned} \tag{3}$$

Here, average transverse leakage is defined by

$$\mathbf{D}^{m}\bar{\mathbf{L}}_{u}^{m} = \sum_{v\neq u}\frac{1}{a_v^m}\left(\mathbf{j}_{vr}^{m+} - \mathbf{j}_{vr}^{m-} - \mathbf{j}_{vl}^{m+} + \mathbf{j}_{vl}^{m-}\right) \tag{4}$$

Depending on the choice of the matrices $\mathbf{M}_{iu}^{m}(i=1,2,3,4)$ defined in Ref. [1], UNM equations can produce various solutions such as NEM solution, ANM solution.

The WRM equations that link the $\mathbf{C}_{iu}^{m}(i=3,4)$ to so many partial currents are not only inconvenient for keeping track of the involved nodes in programming but also inefficient for the numerical computation of the adjoint solution. To avoid this, node-averaged transverse leakage terms are treated as additional unknowns and include Eq.(4) into the forward UNM equations.

Therefore, the set of the nodal forward Eqs. (1), (2), (3), and (4) can be put into the following matrix form with respect to all nodes.

$$\left[\mathbf{H} - \lambda\mathbf{F}\right]\boldsymbol{\Psi} = 0 \tag{5}$$

where

$$\boldsymbol{\Psi} = \left(\bar{\boldsymbol{\phi}}, \mathbf{j}_x^{in}, \mathbf{j}_y^{in}, \mathbf{j}_z^{in}, \mathbf{C}_x, \mathbf{C}_y, \mathbf{C}_z, \bar{\mathbf{L}}_x, \bar{\mathbf{L}}_y, \bar{\mathbf{L}}_z\right)^T$$

2.2 Adjoint Equation for Unified Nodal Method

The transpose of the coefficients matrix defines the mathematical adjoint equations corresponding to the UNM forward equations.

$$\left[\mathbf{H}^T - \lambda\mathbf{F}^T\right]\boldsymbol{\Psi}^* = 0 \tag{6}$$

where

$$\boldsymbol{\Psi}^* = \left(\bar{\boldsymbol{\phi}}^*, \mathbf{j}_x^{in*}, \mathbf{j}_y^{in*}, \mathbf{j}_z^{in*}, \mathbf{C}_x^*, \mathbf{C}_y^*, \mathbf{C}_z^*, \bar{\mathbf{L}}_x^*, \bar{\mathbf{L}}_y^*, \bar{\mathbf{L}}_z^*\right)^T$$

Also, the mathematical adjoint equations, Eq.(6), can be rewritten with respect to a node.

Finally, one can derive the similar iterative procedure to that of the forward UNM.

First, determine $\mathbf{C}_{iu}^{m}(i=3,4)$ from adjoint partial currents.

$$\mathbf{M}_{3u}^{mT}\mathbf{C}_{3u}^{m*} = -\mathbf{Q}_{1u}^{m}\left(\mathbf{j}_{ul}^{m+*} - \mathbf{j}_{ur}^{m-*}\right)$$

$$\mathbf{M}_{4u}^{mT}\mathbf{C}_{4u}^{m*} = \mathbf{Q}_{0u}^{m}\left(\frac{2}{a_u}\bar{\boldsymbol{\phi}}^{m*} + \mathbf{j}_{ul}^{m+*} + \mathbf{j}_{ur}^{m-*}\right) \tag{7}$$

Second, determine adjoint average transverse leakage from the above coefficients, $\mathbf{C}_{iu}^{m}(i=3,4)$.

$$\mathbf{D}^{m}\bar{\mathbf{L}}_{u}^{m*} = -\left(\begin{aligned}&\mathbf{B}_{3ur}^{m-1}\mathbf{D}^{m-1}\mathbf{C}_{3u}^{m-1*} + \mathbf{B}_{3uc}^{m}\mathbf{D}^{m}\mathbf{C}_{3u}^{m*} + \mathbf{B}_{3ul}^{m+1}\mathbf{D}^{m+1}\mathbf{C}_{3u}^{m+1*}\\ &+\mathbf{B}_{4ur}^{m-1}\mathbf{D}^{m-1}\mathbf{C}_{4u}^{m-1*} + \mathbf{B}_{4uc}^{m}\mathbf{D}^{m}\mathbf{C}_{4u}^{m*} + \mathbf{B}_{4ul}^{m+1}\mathbf{D}^{m+1}\mathbf{C}_{4u}^{m+1*}\end{aligned}\right) \tag{8}$$

Third, solve the following equations for adjoint node average flux and adjoint partial currents.

$$\begin{aligned}&\left[\mathbf{A}^{mT} + 12\sum_{u=x,y,z}\frac{1}{a_u}\mathbf{Q}_{0u}^{m}\right]\bar{\boldsymbol{\phi}}^{m*}\\ &= \sum_{u=x,y,z}\left[\mathbf{M}_{2u}^{mT}\mathbf{C}_{4u}^{m*} - 6\mathbf{Q}_{0u}^{m}\left(\mathbf{j}_{ul}^{m+*} + \mathbf{j}_{ur}^{m-*}\right)\right]\end{aligned} \tag{9}$$

$$\begin{aligned}\mathbf{j}_{ul}^{m-*} &= -\frac{1}{a_u}\left(\mathbf{I} + \mathbf{Q}_{2u}^{m} - \mathbf{Q}_{3u}^{m}\right)\bar{\boldsymbol{\phi}}^{m*} + \mathbf{Q}_{3u}^{m}\mathbf{j}_{ul}^{m+*} - \mathbf{Q}_{2u}^{m}\mathbf{j}_{ur}^{m-*}\\ &+\mathbf{M}_{1u}^{m-1T}\mathbf{C}_{3u}^{m-1*} - \mathbf{M}_{1u}^{mT}\mathbf{C}_{3u}^{m*} + \mathbf{M}_{2u}^{m-1T}\mathbf{C}_{4u}^{m-1*} + \mathbf{M}_{2u}^{mT}\mathbf{C}_{4u}^{m*}\\ &-\left(\frac{\bar{\mathbf{L}}_{v}^{m-1*} + \bar{\mathbf{L}}_{w}^{m-1*}}{a_u^{m-1}} - \frac{\bar{\mathbf{L}}_{v}^{m*} + \bar{\mathbf{L}}_{w}^{m*}}{a_u^{m}}\right)\\ \mathbf{j}_{ur}^{m+*} &= -\frac{1}{a_u}\left(\mathbf{I} + \mathbf{Q}_{2u}^{m} - \mathbf{Q}_{3u}^{m}\right)\bar{\boldsymbol{\phi}}^{m*} - \mathbf{Q}_{2u}^{m}\mathbf{j}_{ul}^{m+*} + \mathbf{Q}_{3u}^{m}\mathbf{j}_{ur}^{m-*}\\ &+\mathbf{M}_{1u}^{mT}\mathbf{C}_{3u}^{m*} - \mathbf{M}_{1u}^{m+1T}\mathbf{C}_{3u}^{m+1*} + \mathbf{M}_{2u}^{mT}\mathbf{C}_{4u}^{m*} + \mathbf{M}_{2u}^{m+1T}\mathbf{C}_{4u}^{m+1*}\\ &-\left(\frac{\bar{\mathbf{L}}_{v}^{m+1*} + \bar{\mathbf{L}}_{w}^{m+1*}}{a_u^{m+1}} - \frac{\bar{\mathbf{L}}_{v}^{m*} + \bar{\mathbf{L}}_{w}^{m*}}{a_u^{m}}\right)\end{aligned} \tag{10}$$

Here, all coefficients and response matrices are determined by transposing those of the forward UNM. Therefore, depending on the choice of the transposed matrices, $\mathbf{M}_{iu}^{mT}$, the adjoint solutions of many different nodal computational options can be easily obtained like as the forward UNM.

3. Numerical Results and Conclusion

The validity of adjoint solution method presented in Sec. 2 is examined by comparing mathematical adjoint solution with physical adjoint solution for the two-dimensional International Atomic Energy Agency (IAEA) benchmark problem. The physical adjoint equation can be derived on the UNM principle from physical adjoint equations. Therefore, the mathematical adjoint solution are equal to the physical adjoint solution in homogeneous system like the IAEA benchmark problem.

Table 1 shows the comparison of the forward solution, physical adjoint solution and mathematical adjoint solution for the eigenvalues. It can be shown that all solutions, forward, physical and mathematical, have the same eigenvalues. Furthermore, in comparison with NEM 4Node/FA result, we note that ANM with Analytic Transverse Leakage (ATL) is slightly more accurate than ANM with Quadratic Transverse Leakage (QTL) and NEM is the least accurate.

IAEA 2D		Nodal Option			
		NEM 2x2	NEM 1x1	UANM/QTL (a)	UANM/ATL (b)
K_eff	Forward	1.02961	1.02953	1.02964	1.02962
	Physical Adjoint	1.02961	1.02953	1.02964	1.02962
	Mathematical Adjoint	1.02962	1.02953	1.02964	1.02962

(a) ANM 1x1 with Quadratic Transverse Leakage
(b) ANM 1x1 with Analytic Transverse Leakage

Table 1. Comparison of Effective Multiplication Factors.

In Figure.1, the mathematical adjoint flux for the nodal computational options are compared with the reference, NEM 2x2. Comparison of Figure. 1 also shows the same trend as the previous results.

IAEA2D Thermal Group

1.007 0.70 0.00 0.10	1.770 0.96 −0.28 −0.11	1.965 1.07 −0.10 0.05	1.637 0.79 −0.24 −0.06	0.825 0.12 0.12 0.12	1.267 −0.08 −0.24 −0.16	1.266 −0.39 0.08 0.08	0.923 −1.19 0.00 −0.11
	1.940 0.98 −0.15 0.00	2.000 0.90 −0.10 0.05	1.778 0.79 −0.06 0.06	1.448 0.41 −0.21 −0.14	1.404 0.00 −0.07 0.00	1.289 −0.54 0.08 0.00	0.902 −1.22 0.00 −0.11
		1.987 0.65 −0.25 −0.10	1.820 0.60 −0.11 0.00	1.597 0.44 0.00 0.06	1.451 −0.14 0.07 0.07	1.315 −0.76 0.08 −0.08	0.762 −1.44 0.26 0.00
			1.615 0.50 −0.06 0.00	1.310 0.15 −0.15 −0.08	1.230 −0.33 0.08 0.00	1.027 −1.07 0.19 0.00	
				0.638 −0.47 0.16 0.16	0.925 −0.86 −0.11 −0.32	0.661 −1.82 0.00 −0.30	
					0.641 −1.72 0.00 −0.31		

	k_eff
Reference (a)	1.02962
NEM 1x1	1.02953
UANM/QTL 1x1	1.02964
UANM/ATL 1x1	1.02962

	NEM	ANM/QTL	ANM/ATL
RMS Error	0.865	0.136	0.127

(a) NEM 2x2

Figure 1. Comparison of Mathematical Adjoint Flux

In this paper, we presented a method for determining a mathematical adjoint solution for UNM. The mathematical adjoint equations are derived by transposing the forward equation of UNM and are readily solved for various nodal computational options in the same way as the forward UNM. This adjoint solution method could also be utilized for the multigroup problem, because the multigroup UNM formulation is equal to the form of the two-group model.

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