A High-Order Nodal Method Based on the Function Expansion, Subcell Balances for Even-Parity Transport Problems

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Abstract - In this paper, a new high-order nodal method based on the function expansion, subcell balances for solving the discrete ordinates even-parity transport problems in slab geometry is presented. Two methods are devised to expand the even-parity angular flux : polynomial expansion (four terms including constant) and analytic eigenfunction expansion (five terms including constant particular solution). To derive the coupling equations, the continuity conditions of interface odd-parity angular flux and subcell balances are used. The numerical results are compared with those of diamond difference (DD) and linear moment (LM) methods for the first-order form transport equation. The results show that the method of analytic eigenfunction expansion gives more accurate solutions than DD and LM but that the method of polynomial expansion is less accurate than LM or more accurate than LM (depends on the problems). For S_4 angular quadrature set, it is shown that the method of analytic eigenfuction expansion is an exact differencing scheme (no truncation error).

I. Introduction

In few decades, there have been significant advances[1,2] in the nodal methods for solving the neutron diffusion problems. The methods use the expansion of the neutron flux or the transverse leakages by polynomials or analytic basis functions. These successes lead to some applications of these nodal methods to even-parity or simplified transport equations[3,4]. To our knowledge, there have been no use of exact eigenfunction expansions and subcell balance methods to couple the nodal variables. The subcell balance methods[5,6,7] in devising auxiliary equations have been popularly used in nodal methods for solving discrete ordinates form of the first-order transport equation. In general, it is more difficult to devise accurate differencing schemes in solving second-order form (or even-parity) of the transport equation than in the first-order form. Most of method solving the even-parity transport equation depend on the finite difference method (FDM) and finite element method (FEM). On the other hand, recently, several researchers[8,9,10] have studied to devise highly accurate or exact differencing methods for solving the first-order form of one-group and multi-group transport equation in one-dimensional or two-dimensional geometries.

In this paper, a new high-order nodal method based on the function expansion, subcell balances for solving the discrete ordinates even-parity transport problems in slab geometry is devised. In the method, the even-parity angular flux is expanded by polynomials or analytic eigenfunctions. At present, the polynomial expansion is performed by using four terms including constant term and the analytic eigenfunction expansion is by using dominant four terms and one particular solution term. To derive the nodal coupling equation, the continuity conditions of the interface odd-parity angular flux and the subcell balance conditions are used. To test our method, the method is applied to two simple benchmark problems. The numerical results are compared with those of diamond difference (DD) and

linear moment (LM) methods[11] for the first-order form transport equation. The results show that the method of analytic eigenfunction expansion gives more accurate solutions than DD and LM but that the method of polynomial expansion is less accurate than LM or more accurate than LM. For S_4 angular quadrature set, it is shown that the method of analytic eigenfuction expansion is an exact differencing scheme (no truncation error).

II. Theory and Computational Methodology

Our method starts with the following transport equation of second-order form in slab geometry :

$$-\mu_m \frac{\partial}{\partial x}\left(\frac{\mu_m}{\sigma}\frac{\partial \psi_m^+(x)}{\partial x}\right) + \sigma \psi_m^+(x) = \sigma_s \sum_{n=1}^{N/2} w_n \psi_n^+(x) + q,\tag{1}$$

where w_n is the angular weight normalized to unity over half-range angular domain and ψ^+ represents the even-parity angular flux. In Eq.(1), it is assumed that the scattering is isotropic. The odd-parity angular flux ψ^- is represented in terms of the even-parity angular flux, similarly to Fick's law as follows :

$$\psi_m^-(x) = -\frac{\mu_m}{\sigma}\frac{\partial \psi_m^+(x)}{\partial x}.\tag{2}$$

And the true angular flux is simply given by the arithmetic average of the even- and odd-parity angular fluxes. In fact, this relation is due to the following definitions :

$$\begin{aligned}\psi^+(x,\mu) &= \frac{\psi(x,\mu)+\psi(x,-\mu)}{2},\\ \psi^-(x,\mu) &= \frac{\psi(x,\mu)-\psi(x,-\mu)}{2}.\end{aligned}\tag{3}$$

From the first equation of Eqs.(3), the scalar flux is given by

$$\begin{aligned}\phi(x) &= \frac{1}{2}\int_{-1}^{+1} d\mu \psi(x,\mu) = \int_0^1 d\mu \psi^+(x,\mu)\\ &= \sum_{n=1}^{N/2} w_n \psi_n^+(x).\end{aligned}\tag{4}$$

Therefore, the even-parity transport equation (Eq.(1)) can be solved by considering only angular domain of $\mu > 0$. As the first step of derivation, the even-parity angular flux in a node $[-h/2, h/2]$ is expanded by

$$\psi_m^+(x) = a_m + b_m x + c_m x^2 + d_m x^3\tag{5}$$

for polynomial expansion and for analytic eigenfunction expansion, is by

$$\psi_m^+(x) = a_m \sinh\left(\frac{\sigma x}{\nu_1}\right) + b_m \cosh\left(\frac{\sigma x}{\nu_1}\right) + c_m \sinh\left(\frac{\sigma x}{\nu_2}\right) + d_m \cosh\left(\frac{\sigma x}{\nu_2}\right) + \frac{q}{\sigma_a}.\tag{6}$$

In Eq.(6), ν_1, ν_2 are the first and second dominant eigenvalues of Eq.(1), and they are determined by

$$\sum_{m=1}^{N/2} w_m \phi_\nu(\mu_m) = 1,$$
$$\phi_\nu(\mu_m) = \frac{c}{1 - \frac{\mu_m^2}{\nu^2}},\tag{7}$$

where c means the scattering-to-total ratio. For simplicity, all derivations will be performed for the analytic eigenfunction expansion. Since there are four expansion coefficients in Eq.(6), four nodal

variables are required to be used. At present, the two even-parity interface angular fluxes ($\psi^+_{m,L}$, $\psi^+_{m,R}$) and two subcell average even-parity angular fluxes ($\psi^+_{m,hL}$, $\psi^+_{m,hR}$) are used as the nodal variables. By using Eq.(6), the four nodal variables can be represented by four expansion coefficients. And some simple algebraic procedures lead to the following relations between the nodal variables and expansion coefficients :

$$
\begin{aligned}
b_m &= \alpha_m(\psi^+_{m,L} + \psi^+_{m,R} - \frac{2q}{\sigma}) + \beta_m(\psi^+_{m,hL} + \psi^+_{m,hR} - \frac{2q}{\sigma_a}), \\
d_m &= \alpha_{1m}(\psi^+_{m,L} + \psi^+_{m,R} - \frac{2q}{\sigma}) + \beta_{1m}(\psi^+_{m,hL} + \psi^+_{m,hR} - \frac{2q}{\sigma_a}), \\
a_m &= \gamma_m(\psi^+_{m,R} - \psi^+_{m,L}) + \lambda_m(\psi^+_{m,hR} - \psi^+_{m,hL}), \\
b_m &= \gamma_{1m}(\psi^+_{m,R} - \psi^+_{m,L}) + \lambda_{1m}(\psi^+_{m,hR} - \psi^+_{m,hL}),
\end{aligned}
\tag{8}
$$

where $\alpha, \beta, \gamma, \lambda, \alpha_1, \beta_1, \gamma_1, \lambda_1$ are represented by $\cosh(\frac{\sigma h}{2\nu_i})$ and $\sinh(\frac{\sigma h}{2\nu_i})$. For example, α is given by

$$
\alpha_m = \frac{\frac{4\nu_2}{\sigma h}\sinh(\frac{\sigma h}{2\nu_2})}{\frac{8\nu_2}{\sigma h}\sinh(\frac{\sigma h}{2\nu_2})\cosh(\frac{\sigma h}{2\nu_1}) - \frac{8\nu_1}{\sigma h}\sinh(\frac{\sigma h}{2\nu_1})\cosh(\frac{\sigma h}{2\nu_2})}
\tag{9}
$$

To derive the nodal coupling equations, the following subcell balance equation obtained by integrating Eq.(1) over left half of the node is used :

$$
\mu_m(\psi^-_{m,C} - \psi^-_{m,L}) + \sigma\psi^+_{m,hL}\frac{h}{2} = \sigma_s\phi_{hL}\frac{h}{2} + q_{hL}\frac{h}{2},
\tag{10}
$$

where $\psi^-_{m,C}$ represents the odd-parity flux at the center of the node. The odd-parity flux $\psi^-_{m,L}$ at the left of the node is calculated by using Eq.(2) and (6) as follows :

$$
\begin{aligned}
\psi^-_{m,L} &= -\frac{\mu_m}{\sigma}\frac{\partial\psi^+_m}{\partial x}\Big|_{x=-\frac{h}{2}} \\
&= -\frac{\mu_m}{\nu_1}\cosh(\frac{\sigma h}{2\nu_1})a_m + \frac{\mu_m}{\nu_1}\sinh(\frac{\sigma h}{2\nu_1})b_m - \frac{\mu_m}{\nu_2}\cosh(\frac{\sigma h}{2\nu_2})c_m + \frac{\mu_m}{\nu_2}\sinh(\frac{\sigma h}{2\nu_2})d_m.
\end{aligned}
\tag{11}
$$

The odd-parity flux $\psi^-_{m,C}$ can be calculated similarly and it is given by

$$
\psi^-_{m,C} = -\frac{\mu_m}{\sigma}\frac{\partial\psi^+_m}{\partial x}\Big|_{x=0} = -\frac{\mu_m}{\nu_1}a_m - \frac{\mu_m}{\nu_2}c_m.
\tag{12}
$$

By substituting the expansion coefficients (i.e., Eq.(8)) into Eq.(11) and (12), the odd-parity fluxes can be represented in terms of nodal variables. For example, $\psi^-_{m,L}$ is given by

$$
\psi^-_{m,L} = T_{2m}\psi^+_{m,R} + T_{1m}\psi^+_{m,L} - T_{4m}\psi^+_{m,hR} - T_{3m}\psi^+_{m,hL} - T_{5m}\frac{q}{2\sigma_a},
\tag{13}
$$

where the coefficients T's are given by

$$
\begin{aligned}
T_{1m} &= \frac{\mu_m}{\nu_1}\gamma_m\cosh(\frac{\sigma h}{2\nu_1}) + \frac{\mu_m}{\nu_1}\alpha_m\sinh(\frac{\sigma h}{2\nu_1}) + \frac{\mu_m}{\nu_2}\gamma_{1m}\cosh(\frac{\sigma h}{2\nu_2}) + \frac{\mu_m}{\nu_2}\alpha_{1m}\sinh(\frac{\sigma h}{2\nu_2}) \\
T_{2m} &= -\frac{\mu_m}{\nu_1}\gamma_m\cosh(\frac{\sigma h}{2\nu_1}) + \frac{\mu_m}{\nu_1}\alpha_m\sinh(\frac{\sigma h}{2\nu_1}) - \frac{\mu_m}{\nu_2}\gamma_{1m}\cosh(\frac{\sigma h}{2\nu_2}) + \frac{\mu_m}{\nu_2}\alpha_{1m}\sinh(\frac{\sigma h}{2\nu_2}).
\end{aligned}
\tag{14}
$$

Therefore, the subcell balance equation over left half of the node is given by

$$G_{1m}\psi^+_{m,hR} + G_{2m}\psi^+_{m,hL} = G_{3m}\psi^+_{m,R} + G_{m4}\psi^+_{m,L} + \sigma_s\phi_{hL}\frac{h}{2} + q_{hL}\frac{h}{2} \, . \tag{15}$$

Simiarly, the subcell balance equation over right half of the node can be derived and it is given by

$$G_{2m}\psi^+_{m,hR} + G_{1m}\psi^+_{m,hL} = G_{4m}\psi^+_{m,R} + G_{3m}\psi^+_{m,L} + \sigma_s\phi_{hR}\frac{h}{2} + q_{hR}\frac{h}{2} \, . \tag{16}$$

The next nodal coupling equations are obtained by using the following continuity conditions of the interface odd-parity angular fluxes :

$$\psi^-_{m,R,i} = \psi^-_{m,L,i+1}, \tag{17}$$

where the index i represents the position of the node. By using Eq.(13) and its counter part for the right side, Eq.(17) can be written by

$$(T_{1m,i} + T_{1m,i+1})\psi^+_{m,i+1} + T_{2m,i}\psi^+_{m,i} + T_{2m,i+1}\psi^+_{m,i+2}$$
$$= T_{3m,i}\psi^+_{m,hR,i} + T_{4m,i}\psi^+_{m,hL,i} + T_{5m,i}\frac{2\bar{q}_i}{\sigma_{a,i}} \tag{18}$$
$$+ T_{4m,i+1}\psi^+_{m,hR,i+1} + T_{3m,i+1}\psi^+_{m,hL,i+1} + T_{5m,i+1}2\frac{2\bar{q}_{i+1}}{\sigma_{a,i+1}},$$

where $\psi^+_{m,i+1}$ represents the even-parity angular flux for the direction m at the interface between node i and $i+1$. Up to now, the two nodal coupling equations are derived completely but the boundary conditions must be derived additionally to close the nodal coupling equations. For example, it can be shown that the vacuum condition at the left boundary surface is given by

$$\psi^+_m(0) - \frac{\mu_m}{\sigma}\frac{\partial\psi^+_m(x)}{\partial x}\Big|_{x=0} = 0, \ \mu_m > 0 \, . \tag{19}$$

In Eq.(19), the second term of left side is simply the odd-parity angular flux at the left boundary and therefore, by using Eq.(13), it can be written in terms of nodal variables. The computational procedure of our method can be summarized as follows : first, the half cell scalar fluxes for all nodes are guessed for initial calculation of the scattering source. Second, subcell balance equations are solved with the guessed interface even-parity angular fluxes and the equations representing the continuity condition of interface odd-parity angular fluxes are solved by using previously calculated half cell angular fluxes. Third, new scattering sources for half cells are computed and its convergence is checked.

III. Numerical Results

To verify our new nodal method for solving even-parity transport equation, two benchmark problems are considered. The first problem consists of a homogeneous region having $\sigma = 1$ and $\sigma_s = 0.999$. The size of this problem is 40cm and the vacuum conditions are used at the boundaries. The uniform isotropic inhomogeneous source is located in the region between 10cm and 20cm. The configuration is given in Fig. 1.

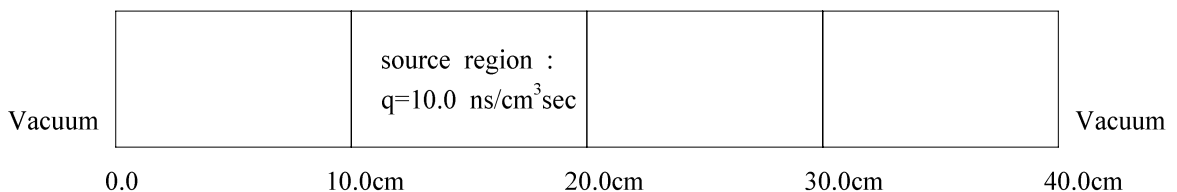| Vacuum		source region : q=10.0 ns/cm^{3}sec			Vacuum
	0.0	10.0cm	20.0cm	30.0cm	40.0cm

Fig. 1 Configuration of the benchmark problem I

This problem is divided into four regions and the accuracy of our method is tested by changing the number of nodes for each region. In Table 1, the results are compared with DD, LM and the infinite medium Green Function (IMGF) Method. It is known that the IMGF method gives the exact solutions of the discrete-ordinates transport problems in slab geometry. All numerical results are obtained by using S_4 angular quadrature set.

Table 1 Comparison of the region average scalar fluxes for benchmark problem I

Region		DD	LM	POL	ANAL	IMGF
1	1[a]	760.764	735.208	716.817	714.603	
	2	724.776	717.347	715.753	714.603	714.605
	3	719.307	715.247	715.203	714.603	
	4	717.106	714.789	714.934	714.603	
2	1	1534.815	1569.575	1690.347	1687.793	
	2	1649.937	1668.934	1688.705	1687.793	1687.796
	3	1671.297	1682.097	1688.259	1687.793	
	4	1678.400	1685.480	1688.051	1687.793	
3	1	1169.092	1136.696	1105.308	1104.530	
	2	1119.362	1109.574	1105.011	1104.530	1104.534
	3	1111.386	1106.015	1104.784	1104.530	
	4	1108.251	1105.109	1104.670	1104.530	
4	1	379.294	368.081	362.117	360.748	
	2	365.247	361.584	361.441	360.748	360.749
	3	362.556	360.885	361.109	360.748	
	4	361.835	360.758	360.948	360.748	

[a]Number of the nodes for each region

The results show that our method (ANAL) gives nearly exact solution and its solution does not depend on the number of nodes (i.e., no truncation error). However, our method with analytic eigenfunction expansion doesn't give the exact solution if angular quadrature sets of higher order than S_4 are used. It is considered that the small discrepancy between our method (ANAL) and IMGF is due to roundoff error or incomplete convergence. And our method with polynomial expansion (POL) converges to the exact solution more rapidly than DD and LM do. The second benchmark problem consists of four different regions. This problem is highly heterogeneous. The configuration, cross sections, and sources of the benchmark problem II are described in Fig. 2.

Vacuum	q=10.0 ns/cm³sec $\sigma = 5$ $\sigma_s = 4.0$	q=0.0 ns/cm³sec $\sigma = 2.0$ $\sigma_s = 0.7$	q=5.0 ns/cm³sec $\sigma = 4.0$ $\sigma_s = 2.0$	q=1.0 ns/cm³sec $\sigma = 1.0$ $\sigma_s = 0.99$	Vacuum

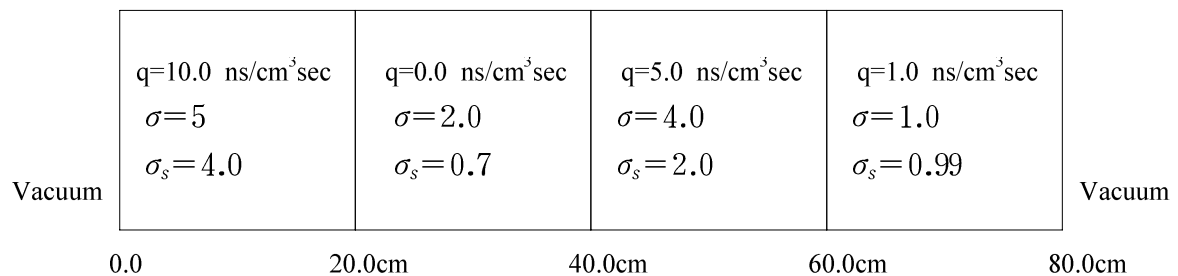0.0   20.0cm   40.0cm   60.0cm   80.0cm

Fig. 2 Configuration of the benchmark problem II

The numerical results are compared in Table 2. The results show that our method with analytic

eigenfunction expansion agrees with the exact solution of IMGF. In fact, the convergence of scattering source iteration for this problem is much more rapid than the benchmark problem I since the scattering ratio is smaller. Therefore, it is considered that the results of ANAL is fully converged and it leads to the exact agreement..

Table 2 Comparison of the region average scalar fluxes results for benchmark problem II

Region		LM	POL	ANAL	IMGF
1	1[a]	9.7461	9.9836	9.8378	9.8378
	2	9.7614	9.9603	9.8378	
	3	9.7697	9.9421	9.8378	
	4	9.7773	9.9269	9.8378	
2	1	1.2046E-04	1.7713E-02	7.9714E-02	7.9714E-02
	2	1.1146E-02	1.9437E-02	7.9714E-02	
	3	1.1053E-02	2.6141E-02	7.9714E-02	
	4	1.0696E-02	3.3236E-06	7.9714E-02	
3	1	2.6621	2.5371	2.6019	2.6019
	2	2.6128	2.5652	2.6019	
	3	2.6064	2.5778	2.6019	
	4	2.6044	2.5849	2.6019	
4	1	28.2440	67.3003	52.6793	52.6793
	2	47.8246	61.5203	52.6793	
	3	50.4607	58.9695	52.6793	
	4	51.3405	57.4119	52.6793	

[a]Number of the nodes for each region

The continuous solution by IMGF is given in Fig. 3. Fig. 3 shows that there are steep gradients at the interfaces between regions. For this problem, all region scalar fluxes for POL except region 2 are less accurate than those of LM. Therefore, it is considered that more detail comparisons of POL and LM are required to investigate their accuracy in future.
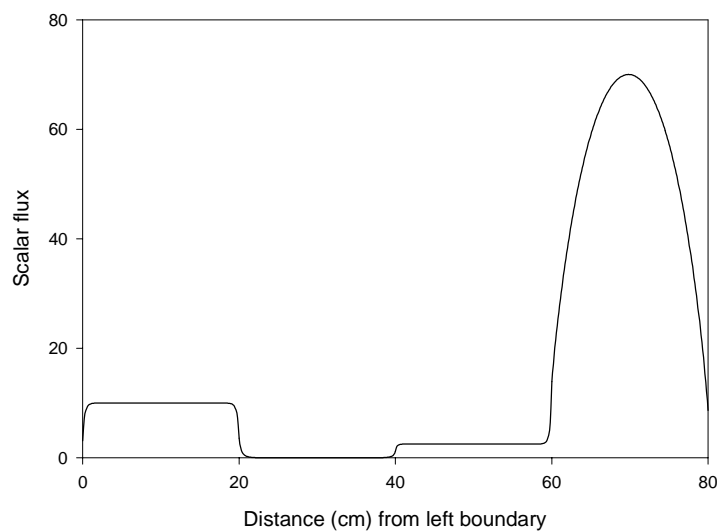

Fig. 3 The scalar flux distribution of the benchmark problem II

IV. Summary and Conclusions

In this paper, a new nodal method for solving the even-parity transport equation in slab geometry is presented. The nodal method is based on the function expansion and subcell balances. Two methods of function expansion are introduced : one is by the polynomial and the other is by analytic eigenfunctions. At present, the number of terms in the expansion is four. From numerical results, it is concluded that our method with analytic eigenfunctions gives the exact solution when S_4 angular quadrature set is used. That is to say, the our method with analytic eigenfunction expansion gives solutions with no truncation error in case of S_4. However, the accuracy of our method with polynomial expansion relative to Linear Moment method depends on problems. For homogeneous problem tested here, the our method with polynomial expansion gave more accurate solution than LM while the accuracy of LM was more good than our method with polynomial expansion. In future work, the acceleration and multi-dimensional extensions of the nodal methods will be studied.

Acknowledgement

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