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NONLINEAR WEIGHTED FLUX METHODS FOR PARTICLE TRANSPORT PROBLEMS IN 2D CARTESIAN GEOMETRY

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ABSTRACT

The family of nonlinear weighted flux methods for solving the transport equation is derived for 2D Cartesian geometry. A linear polynomial weight is considered. An asymptotic diffusion limit analysis is performed on the discretized method. The analysis reveals conditions on the weight necessary for an accurate approximation of the diffusion equation. As a result, we developed a new weighted flux method, the equations of which give rise to the diffusion equation in optically thick diffusive regions. Numerical results are presented to confirm the theoretical results and demonstrate performance of the proposed method.

Key Words: particle transport equation, neutron transport, radiative transfer, iteration methods

1. INTRODUCTION

The nonlinear weighted flux (NWF) methods for solving the transport equation belong to a group of nonlinear projective-iterative (NPI) methods. These are also known as projected discrete ordinates (PDO) methods [1]. The NPI methods are defined by a system of nonlinearly coupled high-order and low-order problems that is equivalent to the original linear transport problem. The equations of NPI methods are closed by a defining of linear-fractional factors. These factors are weakly dependent on the angular flux. NPI methods possess certain advantages for their use in multiphysics applications. NPI methods have some flexibility in coupling, for instance, radiative transfer and hydrodynamics equations. For stability, the low-order equations of these methods need not be discretized consistently with the spatial discretization of the transport equation. Examples of NPI methods are the quasidiffusion (QD) method [2], flux methods [3–5], α-weighted methods [6], nonlinear S_2-like methods [7, 8] and others [1]. These methods differ from each other by the definition of the low-order equations which results in differences in features of these methods. In this paper, we derive new low-order equations of the flux methods such that the resulting discretized NWF method has the desired properties of an accurate approximation of the diffusion equation in the diffusion limit and fast convergence [9].

The low-order problem of the QD method is an elliptic one, i.e. the solution in any spatial point depends on the solution in all other points. However, when particles stream without scattering in some direction, the nature of the relationship of the solution amongst various spatial points is different and based on the properties of the hyperbolic differential operator of the transport equation. The low-order equations of the flux and α-weighted methods are formulated for the partial scalar fluxes and possess such a feature. The flux methods have been used successfully, for instance, to solve electron transport problems with highly anisotropic scattering and radiative transfer problems [10].

In many cases, practical radiative transfer problems contain optically thick diffusive regions in which the leading-order transport solution satisfies the diffusion equation. An asymptotic analysis has been previously developed to assess a discretized method's ability to reproduce the diffusion equation in diffusive regions [9, 11, 12]. This analysis also determines the leading-order boundary condition for the resulting diffusion equation for the case of numerically unresolved boundary layers of the diffusive region. The structure of the flux method equations is similar to that of the transport equation. This asymptotic analysis can be well utilized in the development of the NWF methods with these necessary properties.

Recently, a new parameterized family of NWF methods for the 1D slab geometry transport equation was proposed [13]. The asymptotic diffusion analysis enabled us to determine a particular method of this family the solution of which satisfies a good approximation of both the diffusion equation and asymptotic boundary condition in the diffusive regions. Note that none of the α-weighted nonlinear methods possesses this combination of properties. The convergence properties of this method are close to the properties of the diffusion-synthetic acceleration (DSA) and QD methods.

In this paper, we consider the NWF methods for 2D Cartesian geometry and analyze them to derive a method that possesses a combination of properties necessary for producing accurate numerical solutions of multidimensional transport problems with diffusive regions. We present a NWF method derived with a polynomial weight function whose leading-order solution reproduces an accurate discretization of the diffusion equation in the diffusion limit. Numerical results are presented to illustrate the method's properties.

The remainder of this paper is organized as follows. The family of 2D NWF methods is formulated in Sec. 2. The discretization of the proposed methods is presented in Sec. 3. In Sec. 4, we describe the asymptotic diffusion analysis of the NWF methods in continuous and discrete forms. In Sec. 5, the numerical results are presented. We conclude, in Sec. 6, with a discussion on the developed methods.

2. FORMULATION OF THE FAMILY OF 2D NWF METHODS

Let us consider the one-group steady-state transport equation in 2D Cartesian geometry with isotropic scattering and source:

$$\Omega_x \frac{\partial}{\partial x}\psi(\vec{r},\vec{\Omega}) + \Omega_y \frac{\partial}{\partial y}\psi(\vec{r},\vec{\Omega}) + \sigma_t(\vec{r})\psi(\vec{r},\vec{\Omega}) = \frac{1}{4\pi}\sigma_s(\vec{r})\int_{4\pi}\psi(\vec{r},\vec{\Omega}')d\vec{\Omega}' + \frac{1}{4\pi}q(\vec{r})\,, \quad \vec{r}\in\mathcal{D}\,, \tag{1}$$

$$\psi(\vec{r},\vec{\Omega})\Big|_{\vec{r}\in\partial\mathcal{D}} = \psi^{in}(\vec{r}_b,\vec{\Omega})\,, \quad \vec{\Omega}\cdot\vec{n} < 0\,, \quad \vec{r}_b \in \partial\mathcal{D}\,, \tag{2}$$

where $\mathcal{D} = \{0 \le x \le X,\ 0 \le y \le Y\}$.

To derive the low-order equations of the NWF family of methods, we operate on the transport equation (1) by $\gamma_m \int_{\omega_m} w(\Omega_x,\Omega_y)(\bullet)d\vec{\Omega}$ over spherical angular quadrants ω_m, $m = 1,\dots,4$, where $w(\Omega_x,\Omega_y)$ is a weight function and

$$\gamma_m = \frac{\int_{\omega_m} d\vec{\Omega}}{\int_{\omega_m} w(\Omega_x,\Omega_y)d\vec{\Omega}}\ . \tag{3}$$

The family of 2D NWF methods are then defined by the following high-order problem for the angular flux ψ and low-order problem for the partial scalar fluxes $\phi_m = \int_{\omega_m}\psi d\vec{\Omega}$:

$$\Omega_x \frac{\partial}{\partial x}\psi^{(k+1/2)} + \Omega_y \frac{\partial}{\partial y}\psi^{(k+1/2)} + \sigma_t\psi^{(k+1/2)} = \frac{1}{4\pi}\sigma_s\phi^{(k)} + \frac{1}{4\pi}q\,, \tag{4}$$

$$G_m^{(k+1/2)} = \gamma_m \int\limits_{\omega_m} w(\Omega_x,\Omega_y)\psi^{(k+1/2)} d\vec{\Omega} \Bigg/ \int\limits_{\omega_m} \psi^{(k+1/2)} d\vec{\Omega}\,, \tag{5}$$

$$F_m^{\alpha^{(k+1/2)}} = \gamma_m \int\limits_{\omega_m} |\Omega_\alpha| w(\Omega_x,\Omega_y)\psi^{(k+1/2)} d\vec{\Omega} \Bigg/ \int\limits_{\omega_m} \psi^{(k+1/2)} d\vec{\Omega}\,, \tag{6}$$

$$\alpha = x, y\,, \quad m = 1,\ldots,4\,,$$

$$\frac{\partial}{\partial x}(F_1^{x^{(k+1/2)}}\phi_1^{(k+1)}) + \frac{\partial}{\partial y}(F_1^{y^{(k+1/2)}}\phi_1^{(k+1)}) + \sigma_t G_1^{(k+1/2)}\phi_1^{(k+1)} = \frac{1}{4}(\sigma_s\phi^{(k+1)} + q)\,, \tag{7}$$

$$-\frac{\partial}{\partial x}(F_2^{x^{(k+1/2)}}\phi_2^{(k+1)}) + \frac{\partial}{\partial y}(F_2^{y^{(k+1/2)}}\phi_2^{(k+1)}) + \sigma_t G_2^{(k+1/2)}\phi_2^{(k+1)} = \frac{1}{4}(\sigma_s\phi^{(k+1)} + q)\,, \tag{8}$$

$$-\frac{\partial}{\partial x}(F_3^{x^{(k+1/2)}}\phi_3^{(k+1)}) - \frac{\partial}{\partial y}(F_3^{y^{(k+1/2)}}\phi_3^{(k+1)}) + \sigma_t G_3^{(k+1/2)}\phi_3^{(k+1)} = \frac{1}{4}(\sigma_s\phi^{(k+1)} + q)\,, \tag{9}$$

$$\frac{\partial}{\partial x}(F_4^{x^{(k+1/2)}}\phi_4^{(k+1)}) - \frac{\partial}{\partial y}(F_4^{y^{(k+1/2)}}\phi_4^{(k+1)}) + \sigma_t G_4^{(k+1/2)}\phi_4^{(k+1)} = \frac{1}{4}(\sigma_s\phi^{(k+1)} + q)\,, \tag{10}$$

$$0 \le x \le X,\ 0 \le y \le Y\,,$$

$$\phi^{(k+1)} = \sum_{m=1}^{4} \phi_m^{(k+1)}\,, \tag{11}$$

with the following boundary conditions for the low-order equations (7)-(11):

$$\phi_m^{(k+1)}\Big|_{x=0} = \int\limits_{\omega_m} \psi^{in}\Big|_{x=0} d\vec{\Omega}\,,\ m = 1,4\,,\ 0 \le y \le Y\,, \tag{12}$$

$$\phi_m^{(k+1)}\Big|_{x=X} = \int\limits_{\omega_m} \psi^{in}\Big|_{x=X} d\vec{\Omega}\,,\ m = 2,3\,,\ 0 \le y \le Y\,, \tag{13}$$

$$\phi_m^{(k+1)}\Big|_{y=0} = \int\limits_{\omega_m} \psi^{in}\Big|_{y=0} d\vec{\Omega}\,,\ m = 1,2\,,\ 0 \le x \le X\,, \tag{14}$$

$$\phi_m^{(k+1)}\Big|_{y=Y} = \int\limits_{\omega_m} \psi^{in}\Big|_{y=Y} d\vec{\Omega}\,,\ m = 3,4\,,\ 0 \le x \le X\,. \tag{15}$$

Standard notations are used. k is the iteration index.

The iterative process is defined by the following three stages:

1. A transport sweep to calculate the angular flux $\psi^{(k+1/2)}$ (Eq. (4)).
2. The calculation of the factors $G_m^{(k+1/2)}$ and $F_m^{\alpha^{(k+1/2)}}$ from $\psi^{(k+1/2)}$ (Eqs. (5)-(6)).
3. Solving the low-order problem (Eqs. (7)-(15)) for $\phi_m^{(k+1)}$ using $G_m^{(k+1/2)}$ and $F_m^{\alpha^{(k+1/2)}}$.

On the first iteration ($k = 0$) the transport sweep is not performed. The factors $G_m^{(1/2)}$ and $F_m^{\alpha^{(1/2)}}$ are calculated using an isotropic angular flux.

3. DISCRETIZATION OF THE NWF METHODS

The structure of the operator of the low-order NWF equations has some features that make them similar to the transport equation. This enables one to use transport differencing methods as a basis for development of a discretization of the low-order NWF equations.

We consider orthogonal spatial grids

$$x_{i+1/2} = x_{i-1/2} + \Delta x_i,\ i = 1, \dots, N_x;\ \ x_{1/2} = 0,\ x_{N_x+1/2} = X\,,$$
$$y_{j+1/2} = y_{j-1/2} + \Delta y_j,\ j = 1, \dots, N_y;\ \ y_{1/2} = 0,\ y_{N_y+1/2} = Y\,.$$

The low-order equations are discretized by the lumped bilinear-discontinuous (BLD) method [14, 15]. The BLD approximation of the partial scalar fluxes in the (i, j)-cell is

$$\phi_m(x,y) = \phi_{m,i,j} + \frac{2}{\Delta x_i}(x-x_i)\phi^x_{m,i,j} + \frac{2}{\Delta y_j}(y-y_j)\phi^y_{m,i,j} + \frac{4}{\Delta x_i \Delta y_j}(x-x_i)(y-y_j)\phi^{xy}_{m,i,j}\,, \quad (16)$$

where x_i and y_j are midpoints of the corresponding intervals. The discretized low-order equations of the NWF method are:

$$\nu^x_m \Delta y_j (F^x_{m,i+1/2,j}\phi_{m,i+1/2,j} - F^x_{m,i-1/2,j}\phi_{m,i-1/2,j}) + \nu^y_m \Delta x_i (F^y_{m,i,j+1/2}\phi_{m,i,j+1/2} - F^y_{m,i,j-1/2}\phi_{m,i,j-1/2})$$
$$+ \sigma_{t,i,j} G_{m,i,j}\phi_{m,i,j}\Delta x_i \Delta y_j = \frac{1}{4}\Delta x_i \Delta y_j (\sigma_{s,i,j}\phi_{i,j} + q_{i,j})\,, \quad (17)$$

$$\theta_x \nu^x_m \Delta y_j (F^x_{m,i+1/2,j}\phi_{m,i+1/2,j} + F^x_{m,i-1/2,j}\phi_{m,i-1/2,j} - 2F^x_{m,i,j}\phi_{m,i,j}) + \gamma_y \nu^y_m \Delta x_i (F^y_{m,i,j+1/2}\phi^x_{m,i,j+1/2}$$
$$- F^y_{m,i,j-1/2}\phi^x_{m,i,j-1/2}) + \sigma_{t,i,j} G_{m,i,j}\phi^x_{m,i,j}\Delta x_i \Delta y_j = \frac{1}{4}\Delta x_i \Delta y_j (\sigma_{s,i,j}\phi^x_{i,j} + q^x_{i,j})\,, \quad (18)$$

$$\gamma_x \nu^x_m \Delta y_j (F^x_{m,i+1/2,j}\phi^y_{m,i+1/2,j} - F^x_{m,i-1/2,j}\phi^y_{m,i-1/2,j}) + \theta_y \nu^y_m \Delta x_i (F^y_{m,i,j+1/2}\phi_{m,i,j+1/2}$$
$$+ F^y_{m,i,j-1/2}\phi_{m,i,j-1/2} - 2F^y_{m,i,j}\phi_{m,i,j}) + \sigma_{t,i,j} G_{m,i,j}\phi^y_{m,i,j}\Delta x_i \Delta y_j = \frac{1}{4}\Delta x_i \Delta y_j (\sigma_{s,i,j}\phi^y_{i,j} + q^y_{i,j})\,, \quad (19)$$

$$\delta_x \nu^x_m \Delta y_j (F^x_{m,i+1/2,j}\phi^y_{m,i+1/2,j} + F^x_{m,i-1/2,j}\phi^y_{m,i-1/2,j} - 2F^x_{m,i,j}\phi^y_{m,i,j}) + \delta_y \nu^y_m \Delta x_i (F^y_{m,i,j+1/2}\phi^x_{m,i,j+1/2}$$
$$+ F^y_{m,i,j-1/2}\phi^x_{m,i,j-1/2} - 2F^y_{m,i,j}\phi^x_{m,i,j}) + \sigma_{t,i,j} G_{m,i,j}\phi^{xy}_{m,i,j}\Delta x_i \Delta y_j = \frac{1}{4}\Delta x_i \Delta y_j (\sigma_{s,i,j}\phi^{xy}_{i,j} + q^{xy}_{i,j})\,, \quad (20)$$
$$i = 1, \dots, N_x\,, \quad j = 1, \dots, N_y \quad m = 1, \dots, 4\,,$$

where

$$\nu^x_1 = \nu^x_4 = 1\,, \quad \nu^x_2 = \nu^x_3 = -1\,, \quad (21)$$
$$\nu^y_1 = \nu^y_2 = 1\,, \quad \nu^y_3 = \nu^y_4 = -1\,. \quad (22)$$

The BLD auxiliary equations are given by

$$\phi_{1,i+1/2,j} = \phi_{1,i,j} + \phi^x_{1,i,j}\,, \qquad \phi_{3,i-1/2,j} = \phi_{3,i,j} - \phi^x_{3,i,j}\,,$$
$$\phi^y_{1,i+1/2,j} = \phi^y_{1,i,j} + \phi^{xy}_{1,i,j}\,, \qquad \phi^y_{3,i-1/2,j} = \phi^y_{3,i,j} - \phi^{xy}_{3,i,j}\,,$$
$$\phi_{1,i,j+1/2} = \phi_{1,i,j} + \phi^y_{1,i,j}\,, \qquad \phi_{3,i,j-1/2} = \phi_{3,i,j} - \phi^y_{3,i,j}\,,$$
$$\phi^x_{1,i,j+1/2} = \phi^x_{1,i,j} + \phi^{xy}_{1,i,j}\,, \qquad \phi^x_{3,i,j-1/2} = \phi^x_{3,i,j} - \phi^{xy}_{3,i,j}\,,$$

$$\phi_{2,i-1/2,j} = \phi_{2,i,j} - \phi^x_{2,i,j}\,, \qquad \phi_{4,i+1/2,j} = \phi_{4,i,j} + \phi^x_{4,i,j}\,,$$
$$\phi^y_{2,i-1/2,j} = \phi^y_{2,i,j} - \phi^{xy}_{2,i,j}\,, \qquad \phi^y_{4,i+1/2,j} = \phi^y_{4,i,j} + \phi^{xy}_{4,i,j}\,,$$
$$\phi_{2,i,j+1/2} = \phi_{2,i,j} + \phi^y_{2,i,j}\,, \qquad \phi_{4,i,j-1/2} = \phi_{4,i,j} - \phi^y_{4,i,j}\,,$$
$$\phi^x_{2,i,j+1/2} = \phi^x_{2,i,j} + \phi^{xy}_{2,i,j}\,, \qquad \phi^x_{4,i,j-1/2} = \phi^x_{4,i,j} - \phi^{xy}_{4,i,j}\,. \quad (23)$$

Lumping parameters are denoted by θ_α, γ_α, and δ_α ($\alpha = x, y$). The standard BLD equations are obtained by setting the lumping parameters to 3, 1, and 3, respectively. For mass-lumped BLD, the parameters become 1, 1/3, and 1/3. For fully lumped BLD, the parameters all have values of 1.

The transport equation is approximated by the method of short characteristics [16–18], from which the factors are calculated on vertices. Cell-average factors, $F^\alpha_{m,i,j}$ and $G_{m,i,j}$, are calculated as averages of factors evaluated on the four cell vertices. Face-average factors, $F^\alpha_{m,i+1/2,j}$ and $F^\alpha_{m,i,j+1/2}$, are averages of the two nearest vertex values.

4. ANALYSIS OF ASYMPTOTIC DIFFUSION LIMIT

4.1 NWF Methods in Continuous Form

To meet the diffusion limit, the leading-order solution of the low-order equations (7)-(10) must give rise to the diffusion equation [11, 12]. In order to develop a NWF method that satisfies this condition, we perform an asymptotic diffusion limit analysis of the low-order equations of the NWF methods for general weight $w(\Omega_x, \Omega_y)$ under the assumption that the angular flux is isotropic. Then, the factors are

$$G_m = 1\,, \quad F^\alpha_m = \tilde{F}^\alpha_m\,, \quad \alpha = x, y\,, \quad m = 1, \ldots, 4\,,$$

where

$$\tilde{F}^\alpha_m = \gamma_m \int\limits_{\omega_m} |\Omega_\alpha| w(\Omega_x, \Omega_y) d\vec{\Omega} \bigg/ \int\limits_{\omega_m} d\vec{\Omega}\,. \tag{24}$$

The analysis shows that the leading-order solution of the low-order equations (7)-(10) satisfies the following second-order PDE in the interior of the optically thick diffusive region:

$$\begin{aligned} &-\frac{1}{4}\left(\sum_{m=1}^{4}(\tilde{F}^x_m)^2\right)\frac{\partial}{\partial x}\frac{1}{\sigma_t}\frac{\partial \phi^{[0]}}{\partial x} - \frac{1}{4}\left(\sum_{m=1}^{4}(\tilde{F}^y_m)^2\right)\frac{\partial}{\partial y}\frac{1}{\sigma_t}\frac{\partial \phi^{[0]}}{\partial y} \\ &-\frac{1}{4}\left(\tilde{F}^x_1\tilde{F}^y_1 - \tilde{F}^x_2\tilde{F}^y_2 + \tilde{F}^x_3\tilde{F}^y_3 - \tilde{F}^x_4\tilde{F}^y_4\right)\left(\frac{\partial}{\partial x}\frac{1}{\sigma_t}\frac{\partial \phi^{[0]}}{\partial y} + \frac{\partial}{\partial y}\frac{1}{\sigma_t}\frac{\partial \phi^{[0]}}{\partial x}\right) \\ &+\frac{1}{4}\left(\tilde{F}^x_1 + \tilde{F}^x_4 - \sum_{m=2}^{3}\tilde{F}^x_m\right)\frac{\partial \phi^{[1]}}{\partial x} + \frac{1}{4}\left(\sum_{m=1}^{2}\tilde{F}^y_m - \sum_{m=3}^{4}\tilde{F}^y_m\right)\frac{\partial \phi^{[1]}}{\partial y} + \sigma_a\phi^{[0]} = q\,. \end{aligned} \tag{25}$$

The equation (25) results in the diffusion equation and hence the leading-order solution satisfies the diffusion equation, if the following five conditions are met:

$$\frac{1}{4}\sum_{m=1}^{4}(\tilde{F}^x_m)^2 = \frac{1}{3}\,, \tag{26}$$

$$\frac{1}{4}\sum_{m=1}^{4}(\tilde{F}^y_m)^2 = \frac{1}{3}\,, \tag{27}$$

$$\tilde{F}^x_1\tilde{F}^y_1 - \tilde{F}^x_2\tilde{F}^y_2 + \tilde{F}^x_3\tilde{F}^y_3 - \tilde{F}^x_4\tilde{F}^y_4 = 0\,, \tag{28}$$

$$\tilde{F}^x_1 + \tilde{F}^x_4 - \sum_{m=2}^{3}\tilde{F}^x_m = 0\,, \tag{29}$$

$$\sum_{m=1}^{2} \tilde{F}_m^y - \sum_{m=3}^{4} \tilde{F}_m^y = 0\,. \tag{30}$$

The results of this analysis allow an evaluation of NWF methods with various weights. Note that if a weight satisfies only Eqs. (28)-(30), then Eq. (25) leads to a diffusion-like equation with a wrong diffusion coefficient, D.

Let us consider methods with a general linear weight function of directional cosines

$$w(\Omega_x, \Omega_y) = 1 + \beta_x|\Omega_x| + \beta_y|\Omega_y|\,. \tag{31}$$

For the weight (31) and specified above ranges for the partial fluxes (i.e. ω_m), we get

$$\tilde{F}_m^\alpha = \tilde{F}\,, \quad m = 1, \ldots, 4\,, \tag{32}$$

where

$$\tilde{F} = \frac{\frac{1}{2} + \frac{1}{3}(\beta_x + \frac{2}{\pi}\beta_y)}{1 + \frac{1}{2}(\beta_x + \beta_y)}\,. \tag{33}$$

Note that the use of a general constant term in (31) will not result in a different NWF method.

The above five requirements (26)-(30) are met if the following two conditions on the weight (31) are true:

$$\beta_x = \beta_y = \beta\,, \tag{34}$$

where

$$\beta = \frac{\pi\sqrt{3}(\sqrt{3} - 2)}{2(\pi(\sqrt{3} - 1) - 2)} \approx -2.43\,. \tag{35}$$

The weight (31) and parameter β determine a specific method within the family of NWF methods for which the low-order equations lead to the correct diffusion equation in the diffusion limit provided that the factors are calculated with an isotropic angular flux. The low-order equations of methods with $w = 1$, $w = |\Omega_x| + |\Omega_y|$, and $w = 1 + |\Omega_x| + |\Omega_y|$ give rise to a diffusion-like equation, but with a wrong diffusion coefficient. The values of the diffusion coefficients for these methods are shown in Table I.

Table I. Values of the Diffusion Coefficients (D) for Specific NWF Methods

Weight	$w = 1$	$w{=}\lvert\Omega_x\rvert{+}\lvert\Omega_y\rvert$	$w{=}1{+}\lvert\Omega_x\rvert{+}\lvert\Omega_y\rvert$	$w{=}1{+}\beta(\lvert\Omega_x\rvert{+}\lvert\Omega_y\rvert)$
D	$\frac{1}{4\sigma_t}$	$(\frac{\pi+2}{3\pi})^2\frac{1}{\sigma_t} \approx \frac{1}{3.36\sigma_t}$	$(\frac{4+5\pi}{12\pi})^2\frac{1}{\sigma_t} \approx \frac{1}{3.66\sigma_t}$	$\frac{1}{3\sigma_t}$

4.2 NWF Methods in Discretized Form

We now perform an asymptotic diffusion limit analysis of the NWF methods approximated by means of the discretization described above (see Sec. 3) on a uniform rectangular spatial grid. The analysis showed that the equation for the leading-order solution can be reduced to a diffusion-like equation provided that in the cells at the interior of the interfaces of the thick diffusive regions, cell-average factors and downstream face-average factors are defined by the corresponding downstream vertex value, namely, given by:

$$\begin{aligned} G_{1,i,j} &= G_{1,i+1/2,j+1/2} \ , \\ G_{2,i,j} &= G_{2,i-1/2,j+1/2} \ , \\ G_{3,i,j} &= G_{3,i-1/2,j-1/2} \ , \\ G_{4,i,j} &= G_{4,i+1/2,j-1/2} \ , \end{aligned} \tag{36}$$

$$\begin{aligned} F^{\alpha}_{1,i,j} &= F^{\alpha}_{1,i+1/2,j} = F^{\alpha}_{1,i,j+1/2} = F^{\alpha}_{1,i+1/2,j+1/2} \ , \\ F^{\alpha}_{2,i,j} &= F^{\alpha}_{2,i-1/2,j} = F^{\alpha}_{2,i,j+1/2} = F^{\alpha}_{2,i-1/2,j+1/2} \ , \\ F^{\alpha}_{3,i,j} &= F^{\alpha}_{3,i-1/2,j} = F^{\alpha}_{3,i,j-1/2} = F^{\alpha}_{3,i-1/2,j-1/2} \ , \\ F^{\alpha}_{4,i,j} &= F^{\alpha}_{4,i+1/2,j} = F^{\alpha}_{4,i,j-1/2} = F^{\alpha}_{4,i+1/2,j-1/2} \ . \end{aligned} \tag{37}$$

If these conditions are met, then the low-order NWF equations discretized by the BLD method lead to the same discrete equation for the leading-order solution as the BLD discretization of the transport equation [12]. However, the resulting discretized diffusion equation has the diffusion coefficient

$$D = \frac{\tilde{F}^2}{\sigma_t} \,, \tag{38}$$

and hence in general it is not a correct one. In case of the weight $w(\Omega_x, \Omega_y) = 1 + \beta(|\Omega_x| + |\Omega_y|)$, we have $\tilde{F}^2 = \frac{1}{3}$ and obtain the right diffusion coefficient.

We now analyze the behavior of the discretized NWF methods in the presence of a boundary layer that is not resolved by the spatial grid. The asymptotic analysis of the boundary-layer solution of the transport equation in the differential form showed that the leading-order scalar flux meets the following boundary condition [20]:

$$\phi^{[0]}(X, y) = 2 \int_{\vec{n}\cdot\vec{\Omega}<0} W(|\vec{n}\cdot\vec{\Omega}|)\psi_{in}(X, y, \vec{\Omega})d\vec{\Omega} \,, \tag{39}$$

$$W(\mu) = \frac{\sqrt{3}}{2}\mu H(\mu) \approx 0.956\mu + 1.565\mu^2 \,, \tag{40}$$

where $H(\mu)$ is the Chandrasekhar H-function for a purely scattering medium.

Let us consider the boundary condition at $x = X$, where $\vec{n} = \vec{e}_x$. The analysis of the discretized NWF methods revealed that on the boundary of an optically thick diffusive region the leading-order scalar flux is defined by

$$\phi^{[0]}_{N_x,j} = \frac{2\pi \sum\limits_{\vec{n}\cdot\vec{\Omega}_m<0} \left[w(|\Omega_{x,m}|, |\Omega_{y,m}|)|\Omega_{x,m}|\right] \psi_{in}(\vec{\Omega}_m)\zeta_m}{\sum\limits_{m\in\omega_1} w(|\Omega_{x,m}|, |\Omega_{y,m}|)|\Omega_{x,m}|\zeta_m} \,, \tag{41}$$

where ζ_m are quadrature weights. The equation (41) approximates the following boundary relationship in a continuous form:

$$\phi^{[0]}(X, y) = 2 \int_{\vec{n}\cdot\vec{\Omega}<0} \widetilde{W}(|\Omega_x|, |\Omega_y|)\psi_{in}(X, y, \vec{\Omega})d\vec{\Omega} \,, \tag{42}$$

where

$$\widetilde{W}(|\Omega_x|, |\Omega_y|) = \frac{\pi w(|\Omega_x|, |\Omega_y|)|\Omega_x|}{\int_{\omega_1} w(|\Omega_x|, |\Omega_y|)|\Omega_x| d\vec{\Omega}} \,. \tag{43}$$

The asymptotic analysis of other boundaries, for instance at $y = 0$, results in a similar expression.

We now examine the resulting weight function in the boundary condition, $\widetilde{W}(|\Omega_x|, |\Omega_y|)$, for various NWF methods. For the NWF method with $w(\Omega_x, \Omega_y) = 1$ (the first flux method), we get

$$\widetilde{W}(|\Omega_x|) \quad = \quad 2|\Omega_x| \ . \tag{44}$$

For the case $w(\Omega_x, \Omega_y) = |\Omega_x| + |\Omega_y|$, the boundary weight function is

$$\begin{aligned} \widetilde{W}(|\Omega_x|, |\Omega_y|) &= \frac{3\pi}{2+\pi}[|\Omega_x|^2 + |\Omega_y||\Omega_x|] \\ &\approx 1.833[|\Omega_x|^2 + |\Omega_y||\Omega_x|] \ . \end{aligned} \tag{45}$$

The weight $w(\Omega_x, \Omega_y) = 1 + |\Omega_x| + |\Omega_y|$ results in the boundary weight function

$$\begin{aligned} \widetilde{W}(|\Omega_x|, |\Omega_y|) &= \frac{6\pi}{5\pi+4}[|\Omega_x| + |\Omega_x|^2 + |\Omega_y||\Omega_x|] \\ &\approx 0.956[|\Omega_x| + |\Omega_x|^2 + |\Omega_y||\Omega_x|] \ . \end{aligned} \tag{46}$$

If $w(\Omega_x, \Omega_y) = 1 + \beta\,(|\Omega_x| + |\Omega_y|)$, we have

$$\begin{aligned} \widetilde{W}(|\Omega_x|, |\Omega_y|) &= \left[\frac{1}{2} + \beta(\frac{2+\pi}{3\pi})\right]^{-1} \Big(|\Omega_x| + \beta|\Omega_x|^2 + \beta|\Omega_y||\Omega_x|\Big) \\ &\approx -1.209|\Omega_x| + 2.942|\Omega_x|^2 + 2.942|\Omega_y||\Omega_x| \ . \end{aligned} \tag{47}$$

The transport equation's boundary weight function (40) depends only on $\mu = |\vec{n} \cdot \vec{\Omega}|$, which for the boundary considered is $|\Omega_x|$. Note that the resulting boundary weight functions for the considered weights, $w(\Omega_x, \Omega_y)$, each differ from the polynomial approximation of $W(\mu)$. Higher order polynomial weights may be considered, but they are not necessary to produce the asymptotic diffusion equation and will introduce third-order and higher terms into the asymptotic boundary condition that do not exist in the analytic result of the transport equation. The following section presents numerical results that enable one to compare and analyze the properties of different NWF methods.

5. NUMERICAL RESULTS

We present numerical results of two test problems to demonstrate the performance of the proposed 2D NWF method with weight $w(\Omega_x, \Omega_y) = 1 + \beta(|\Omega_x| + |\Omega_y|)$. The first problem is designed to test the diffusion limit performance of the method in the interior of a diffusive region. The second problem investigates both the diffusion limit and the boundary condition properties of the method. We also show the results for the NWF methods with weights $w(\Omega_x, \Omega_y) = 1$, $w(\Omega_x, \Omega_y) = |\Omega_x| + |\Omega_y|$ and $w(\Omega_x, \Omega_y) = 1 + |\Omega_x| + |\Omega_y|$.

Note that the factors in the NWF methods involve integration over individual quadrants of the angular flux multiplied by polynomials of directional cosines. Taking into account this fact, we use Gauss-type quadratures [19], namely, the compatible quadruple-range quadrature with an equal number of azimuthal angles on each polar cone.

Problem 1

We consider a unit square having $\sigma_t = 1/\varepsilon$, $\sigma_a = \varepsilon$, and $q = \varepsilon$ for $\varepsilon = 10^{-2}, 10^{-3}, 10^{-4}, 10^{-5}$ [12]. Note that as $\varepsilon \to 0$ the domain becomes more and more diffusive. A uniform spatial mesh of 19x19 equal cells is used with vacuum boundary conditions. The angular discretization is 9 directions per octant, 3 per polar level. A relative pointwise convergence criterion of 10^{-8} is used.

Tables II and III show measures of the error of the NWF methods' solutions in Problem 1 as compared to the fine-mesh numerical solution obtained by the QD method. Note that the low-order equations of the QD method give rise to the diffusion equation in diffusive regions. The low-order QD equations are discretized by means of a finite-volume method of second-order accuracy. The QD solution accurately reproduces the solution of this problem. Relative errors of the cell-average scalar flux in the cell located at the center of the domain are listed in Table II. The relative errors of the solution in the L_2-norm are shown in Table III. These results demonstrate that the NWF method with the weight $w(\Omega_x, \Omega_y) = 1 + \beta(|\Omega_x| + |\Omega_y|)$ reproduces the maximum of the solution with small errors, especially in case of extremely diffusive regions. The proposed method also has the smallest relative errors in the L_2 norm. Larger errors of the NWF method with other weights $w(\Omega_x, \Omega_y)$ are explained by the fact that the equations of these methods lead to the diffusion equation with a wrong diffusion coefficient (Eq.(38) and Table I) in the interior of diffusive regions.

Problem 2

We consider a boundary layer problem $0 \leq x, y \leq 11$ having $\sigma_t = \sigma_a = 2$, $\Delta x = 0.1$, and $q = 0$ from $0 \leq x \leq 1$ and $\sigma_t = \sigma_s = 100$, $\Delta x = 1$, and $q = 0$ from $1 \leq x \leq 11$ ($\Delta y = 1$ everywhere). There is an isotropic incoming angular flux with magnitude $\frac{1}{2\pi}$ on the left boundary and vacuum on the rest. The angular quadrature set and convergence criterion are the same as in Problem 1. This problem tests a method's ability to reproduce an accurate diffusion solution in the interior of a diffusive region with a spatially unresolved boundary layer.

Figure 1 shows the overall performance of the methods in an unresolved boundary layer problem. The scalar flux from the low-order problem along the middle of the spatial domain at $y = 5.5$ is plotted where the cell-average values are displayed in solid and the face-average values are in outline form. The red curve represents the fine-mesh solution obtained by the QD method. Figure 2 demonstrates the absolute value of the relative errors of the low-order scalar flux with respect to the fine mesh solution. Note that at the right boundary (x=11) the solution is very small ($\phi = 3.724 \times 10^{-5}$). It results in an increase of the relative error at x=11. The presented results show that the NWF method with the smallest errors in the diffusive region with highly anisotropic angular flux coming from the purely absorbing region is the method with the weight $w = 1 + \beta(|\Omega_x| + |\Omega_y|)$.

6. CONCLUSIONS

A parameterized family of nonlinear weighted flux methods for solving particle transport problems in 2D Cartesian geometry has been considered. The properties of these methods for transport problems with isotropic scattering have been analyzed in differential and discretized form. Independent schemes to discretize the low-order and high-order (transport) equations are used. The performed analysis revealed a method with a particular linear weight function the low-order equations of which lead to the diffusion equation in the asymptotic diffusion limit. The resulting low-order NWF equations are discretized with the

Table II. Problem 1: Relative Errors of the Cell-Average Scalar Flux in the Cell Located at the Center of the Domain

Weight	$w = 1$	$w{=}\lvert\Omega_x\rvert{+}\lvert\Omega_y\rvert$	$w{=}1{+}\lvert\Omega_x\rvert{+}\lvert\Omega_y\rvert$	$w{=}1{+}\beta(\lvert\Omega_x\rvert{+}\lvert\Omega_y\rvert)$
$\varepsilon = 10^{-2}$	2.57E-1	1.02E-1	1.76E-1	8.49E-3
$\varepsilon = 10^{-3}$	2.70E-1	9.97E-2	1.81E-1	-7.98E-4
$\varepsilon = 10^{-4}$	2.71E-1	1.00E-1	1.81E-1	-6.02E-4
$\varepsilon = 10^{-5}$	2.71E-1	1.00E-1	1.81E-1	-5.81E-4

Table III. Problem 1: Relative Errors of the Scalar Flux in L_2 Norm

Weight	$w = 1$	$w{=}\lvert\Omega_x\rvert{+}\lvert\Omega_y\rvert$	$w{=}1{+}\lvert\Omega_x\rvert{+}\lvert\Omega_y\rvert$	$w{=}1{+}\beta(\lvert\Omega_x\rvert{+}\lvert\Omega_y\rvert)$
$\varepsilon = 10^{-2}$	2.32E-1	8.56E-2	1.55E-1	1.81E-2
$\varepsilon = 10^{-3}$	2.54E-1	8.82E-2	1.67E-1	1.96E-2
$\varepsilon = 10^{-4}$	2.56E-1	8.90E-2	1.68E-1	1.99E-2
$\varepsilon = 10^{-5}$	2.56E-1	8.91E-2	1.68E-1	1.99E-2

lumped BLD method. The convergence rates of the proposed iterative method are similar to those of the QD and DSA methods. We now work on further analysis and development of the NWF methods.

The proposed NWF method that meets the diffusion limit can be used for developing approximate mathematical models for radiative transfer and particle transport that are similar to the Variable Eddington Factor (VEF) approach [21]. The VEF methods are based on a set of low-order equations for moments of the angular flux and some *apriori* closure relationships, for instance, Levermore-Pomraning or Minerbo closures [22, 23]. For some class of transport problems, these approximate models can be more accurate than the flux-limited diffusion model or P_1 theory. The low-order NWF equations can be used in combination with, for example, Minerbo closure to derive a model with new features. This area of application of the NWF methods in 1D and 2D requires further studies.

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REFERENCES

[1] M.L. Adams and E.W. Larsen, Fast Iterative Methods for Discrete-Ordinates Particle Transport Calculations, *Prog. Nucl. Energy*, **40**, pp. 3-159 (2002).

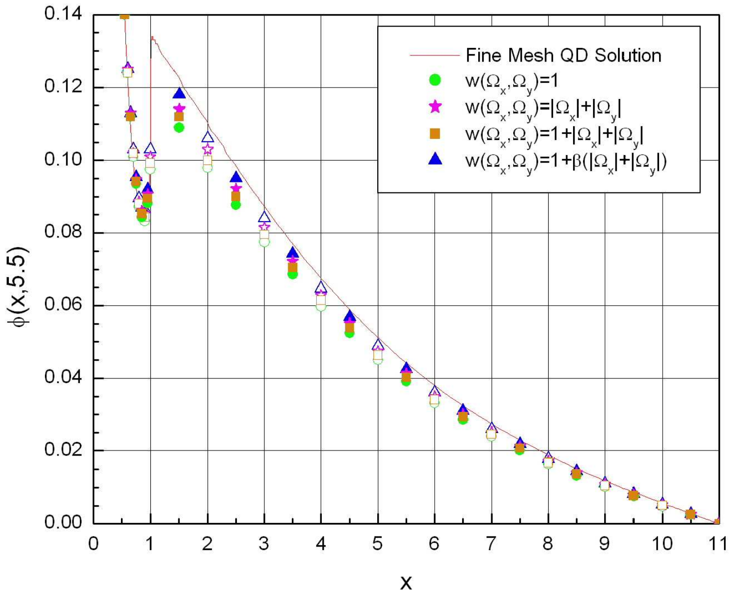

Figure 1. Problem 2: Cell Average and Cell Face Total Low-Order Scalar Flux.

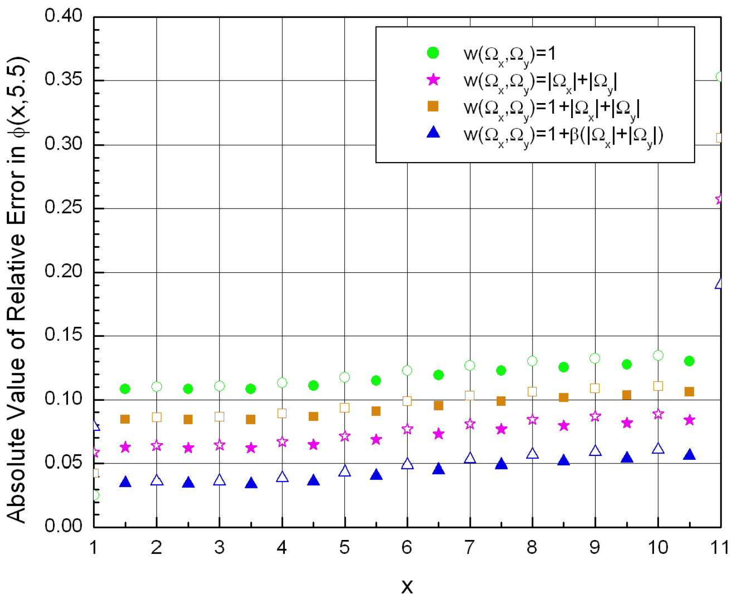

Figure 2. Problem 2: Absolute Value of Relative Errors of the Scalar Flux versus QD Fine Mesh Solution of Figure 1.

[2] V.Ya. Gol'din, A Quasi-Diffusion Method for Solving the Kinetic Equation, *USSR Comp. Math. and Math. Phys.* **4**, pp. 136-149 (1964).

[3] T.A. Germogenova, Convergence of Some Approximate Methods of Solving the Transport Equation, *Soviet Mathematics - Doklady* **9**, pp. 855 (1968).

[4] V.Ya. Gol'din, G.V. Danilova and B.N. Chetverushkin, Approximate Method of Solving the Time-Dependent Kinetic Equation, in *Computational Methods in Transport Theory* (Atomizdat, Moscow, 1969) pp. 50-57 (in Russian).

[5] V.V. Gorskii and S.T. Surzhikov, Use of the Semimoment Method to Solve the Shock Layer Radiative Heat-Transfer Problem, *J. of Eng. Physics*, **42**, No. 1, pp. 108 (1982).

[6] D.Y. Anistratov and E. W. Larsen, "Nonlinear and Linear α-Weighted Methods for Particle Transport Problems," *J. of Computational Physics*, **173**, pp. 664-684 (2001).

[7] M.L. Adams, New Nonlinear Methods for Linear Transport Calculations, in *Proceedings of Joint International Conference on Mathematical Methods and Supercomputing in Nuclear Applications, April 19-23, 1993, Karlsruhe, Germany* pp. 683-694.

[8] S.G. Hong and N.Z. Cho, "A Rebalance Approach to Nonlinear Iteration for Solving the Neutron Transport Equation," *Ann. Nucl. Energy*, **24**, 147 (1997).

[9] E. W. Larsen, "Asymptotic Solutions of Numerical Transport Problems in Optically Thick, Diffusive Regimes II," *J. of Computational Physics*, **83**, 212 (1989).

[10] V.Ya. Goldin, V.A. Kuzyuk, and A.K. Rakhmatulina, "Nonlinear Method of Electron Transport Calculation," *USSR Comp. Math. and Math. Phys.*, **16**, No. 2, 131 (1976).

[11] E. W. Larsen, "The Asymptotic Diffusion Limit of Discretized Transport Problems," *Nucl. Sci. Eng.*, **112**, 336 (1992).

[12] M.L. Adams, Discontinuous Finite Element Transport Solutions in Thick Diffusive Problems, *Nuclear Science and Engineering*, **137**, pp. 298-333 (2001).

[13] L. Roberts and D.Y. Anistratov, "Nonlinear Weighted Flux Methods for Particle Transport Problems," Proceedings of *M&C 2005, International Conference on Mathematics and Computations, Supercomputing, Reactor Physics and Nuclear Biological Applications,* American Nuclear Society Topical Meeting of M&C Division, Avignon, France, September, 2005, 10 pp.

[14] M.L. Adams and W.R. Martin, "Diffusion Synthetic Acceleration of Discontinuous Finite Element Transport Iterations," *Nuclear Science and Engineering*, **111**, 145 (1992).

[15] J.E. Morel, J.E. Dendy, Jr., and T.A. Waring, "Diffusion-Accelerated Solution of the Two-Dimensional S_n Equations with Bilinear-Discontinuous Differencing," *Nuclear Science and Engineering*, **115**, 304-319 (1993).

[16] V.Ya. Gol'din, "Characteristic Difference Scheme for Non-Stationary Kinetic Equation," *Soviet Mathematics - Doklady*, **1**, 902 (1960).

[17] V.Ya. Gol'din, N.N. Kalitkin , and T.V. Shishova, "Nonlinear Difference Schemes for Hyperbolic Equations," *USSR Comp. Math. and Math. Phys.* **5**, 229 (1968).

[18] K.Takeuchi, "A Numerical Method for Solving the Neutron Transport Equation in Finite Cylindrical Geometry," *J. Nucl. Sci.*, **6**, 446 (1969).

[19] I.K. Abu-Shumays, Angular Quadratures for Improved Transport Computations, *Transport Theory Statist. Phys.*, **30**, pp. 169-204 (2001).

[20] K.M. Case and P.E. Zweifel, **Linear Transport Theory**, Addison-Wesley, Reading, MA (1967).

[21] C.D. Levermore, “Relating Eddington Factors to Flux Limiters,” *J. Quant. Spectrosc. Radiat. Transfer*, **31**, 149-160, (1984)

[22] C.D. Levermore and G.C. Pomraning, “A Flux-Limited Diffusion Theory,” *Astrophys. J.*, **248**, 321-334, (1981).

[23] G.N. Minerbo, “Maximum Entropy Eddington Factors,” *J. Quant.Spectrosc. Radiat. Transfer*, **20**, 541-545 (1978).