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Acceleration of the Nonlinear Corner-Balance Scheme by the Averaged Flux Method

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Recently, several nonlinear spatial discretzation methods have been developed for the linear Boltzmann transport equation. One of these is the highly accurate nonlinear corner-balance (NLCB) method, which yields a strictly positive solution. Because the discrete NLCB scheme is algebraically nonlinear, special iterative methods are needed to solve it efficiently. In this paper, we describe a fast new iterative algorithm, based on the nonlinear averaged flux method, for solving the discrete NLCB equations. We present numerical results that illustrate the efficiency of the new algorithm.
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1. INTRODUCTION

The linear Boltzmann equation describes the interaction of radiation (for example, neutrons) with matter. Linearity follows if the neutrons are sufficiently rarefied that they interact mainly with the atoms in the background system, not with themselves. There now exists a group of nonlinear spatial discretization schemes for the linear Boltzmann transport equation. Some of these are the characteristic method with nonlinear interpolation [1], the adaptive weighted diamond-differencing (AWDD) method [2, 3], the exponential method [4], the nonlinear characteristic (NLC) scheme [5, 6], the exponential characteristic (EC) method [7], and the nonlinear corner-balance (NLCB) method [8]. Most of these methods generate very accurate numerical transport solutions. In this paper we consider the fourth-order NLCB method, which is strictly positive and very accurate on coarse spatial grids, especially for deep penetration problems. To solve the NLCB equations, an iterative algorithm must be used. The simplest iterative algorithm is the source iteration (SI) method, which converges too slowly for many important problems. A variety of iterative acceleration methods have been developed for linear transport differencing schemes, but because of the nonlinear nature of the NLCB equations, a special algorithm is needed. In this paper, we develop such an algorithm for the NLCB scheme and demonstrate its effectiveness.

Specifically, we present an iteration algorithm based on the nonlinear averaged flux (AF) method [9, 10], also known as the first-flux (FF) method [11]. The AF method is defined by a nonlinear system of equations with two parts: (i) the transport equation and (ii) low-order equations. The low-order equations are derived by integrating the transport equation over certain intervals of the angular variable. The resulting system of angle-independent equations is closed by special linear-fractional functionals that are weakly dependent on the transport solution. The stability of these functionals with respect to the variation of the solution during iterations yields high convergence rates. The AF method is a member of a class of quasi-projective (QP) methods [11, 12], also known as projected discrete ordinates (PDO) methods [13]. The quasi-diffusion [14] (QD), second-flux [15], and α-weighted acceleration [16] methods are other examples of QP (or PDO) methods. These methods differ by the form of the low-order problem, which comes from integrating the transport equation over various intervals with different weight functions. Unlike the diffusion synthetic acceleration (DSA) method [13], the AF method does not require consistently discretized transport and low-order equations. However, inconsistent differencing produces a converged solution that differs from the unaccelerated solution unless the mesh is sufficiently fine. This different solution is still a legitimate discretized transport solution and may be even more accurate than the unaccelerated one.

In this paper we develop a ''pure'' acceleration method for the NLCB scheme, using consistent discretizations, for planar-geometry transport problems. To begin, we apply the AF method to the discrete NLCB scheme and derive the corresponding discrete low-order problem. The discrete NLCB equations are nonlinear; hence, the resulting low-order equations are also nonlinear in the same way. To cope with this nonlinearity, we apply a Newton's linearization to the low-order difference equations. The linearized low-order problem is solved by Newton's method. Thus, the main computational work arising from the non-

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linearity of the NLCB method is performed in the inexpensive low-order problem. The resulting acceleration method converges very rapidly. The extension to multiple space dimensions is straightforward, but efficiently obtaining the solution of the linearized low-order equations may become problematic.

Earlier the AF method was used for acceleration of the NLC method by T. Wareing, W. Walters and J. Morel [17]. The spatially nonlinear low-order problem for the NLC method was derived by means of the AF method. This nonlinear problem was linearized, but Newton's iteration method was not used to solve the linearized low-order equations. That is, the algorithm [17] is equivalent to performing one Newton's iteration on the low-order equations after each high-order sweep. T. Wareing, W. Walters and J. Morel also use a different approach based on the DSA method [18], where the NLC method is first linearized with respect to certain parameters. Then, the resulting linear transport problem is solved by means of the DSA method, and the parameters are updated using Newton's method.

The remainder of this paper is organized as follows. In Sec. 2 we describe the NLCB method. In Sec. 3 we formulate the new nonlinear acceleration method for the NLCB method. In Sec. 4 we present numerical results, which include comparisons with the NLC scheme accelerated by the AF and DSA methods [17, 18]. We also demonstrate the accuracy of the considered NLCB scheme compared to the diamond-differencing (DD) method [19]. In Sec. 5 we conclude with a brief discussion.

2. FORMULATION OF THE NONLINEAR CORNER-BALANCE METHOD

Let us consider the following single-group planar-geometry transport problem with isotropic scattering and source:

$$\mu \frac{\partial}{\partial x}\psi(x,\mu) + \sigma_t(x)\psi(x,\mu) = \frac{1}{2}(\sigma_s(x)\phi(x) + Q(x)), \quad (1)$$

$$-1 \le \mu \le 1, 0 \le x \le L,$$

$$\phi(x) = \int_{-1}^{1} \psi(x,\mu)\, d\mu, \quad (2)$$

with reflective left boundary

$$\psi(0,\mu) = \psi(0,-\mu), 0 < \mu \le 1, \quad (3)$$

and with a prescribed incident angular flux on the right boundary

$$\psi(L,\mu) = \psi^{in}(\mu), -1 \le \mu < 0. \quad (4)$$

Here, $\psi(x, \mu)$ and $\phi(x)$ are the angular and scalar fluxes, $Q(x)$ is the interior source, and $\sigma_t(x)$ and $\sigma_s(x)$ are the total and scattering cross sections.

To formulate the NLCB method [8], we define a spatial mesh $\{x_{i+1/2}, i = 0, ..., N_x, x_{1/2} = 0, x_{N_x+1/2} = L\}$ and angular quadrature set $\{\mu_m, w_m, m = 1, ..., N_\mu\}$. We assume that cross sections and source are piecewise constant on each spatial cell. The NLCB method consists of the half-cell balance (HCB) equations coupled with characteristic equations

$$\mu_m(\psi_{m,i} - \psi_{m,i-1/2}) + \frac{1}{2}\sigma_{t,i}\psi_{L,m,i}h_i = \frac{1}{4}(\sigma_{s,i}\phi_{L,i} + Q_i)h_i, \quad (5)$$

$$\mu_m(\psi_{m,i+1/2} - \psi_{m,i}) + \frac{1}{2}\sigma_{t,i}\psi_{R,m,i}h_i = \frac{1}{4}(\sigma_{s,i}\phi_{R,i} + Q_i)h_i, \quad (6)$$

$$i = 1, ..., N_x, m = 1, ..., N_\mu,$$

$$\phi_{L,i} = \sum_{m=1}^{N_\mu} \psi_{L,m,i}w_m, \phi_{R,i} = \sum_{m=1}^{N_\mu} \psi_{R,m,i}w_m, \quad (7)$$

$$\psi_{m,i} = \psi_{m,i+1/2}e^{\sigma_{t,i}h_i/(2\mu_m)} + \frac{1}{2\mu_m}\int_{x_{i+1/2}}^{x_i} (\sigma_{s,i}\tilde{\phi}_i(x) + Q_i)e^{-\sigma_{t,i}(x_i - x)/\mu_m}\, dx, \quad (8)$$

$$\psi_{m,i-1/2} = \psi_{m,i}e^{\sigma_{t,i}h_i/(2\mu_m)} + \frac{1}{2\mu_m}\int_{x_i}^{x_{i-1/2}} (\sigma_{s,i}\tilde{\phi}_i(x) + Q_i)e^{-\sigma_{t,i}(x_{i-1/2} - x)/\mu_m}\, dx, \quad (9)$$

$$i = 1, ..., N_x, -1 \le \mu_m < 0,$$

$$\psi_{m,i} = \psi_{m,i-1/2}e^{-\sigma_{t,i}h_i/(2\mu_m)} + \frac{1}{2\mu_m}\int_{x_{i-1/2}}^{x_i} (\sigma_{s,i}\tilde{\phi}_i(x) + Q_i)e^{-\sigma_{t,i}(x_i - x)/\mu_m}\, dx, \quad (10)$$

$$\psi_{m,i+1/2} = \psi_{m,i}e^{-\sigma_{t,i}h_i/(2\mu_m)} + \frac{1}{2\mu_m}\int_{x_i}^{x_{i+1/2}} (\sigma_{s,i}\tilde{\phi}_i(x) + Q_i)e^{-\sigma_{t,i}(x_{i+1/2} - x)/\mu_m}\, dx, \quad (11)$$

$$i = 1, ..., N_x, 0 < \mu_m \le 1,$$

where

$$h_i = x_{i+1/2} - x_{i-1/2}, x_i = \frac{1}{2}(x_{i+1/2} + x_{i-1/2}). \quad (12)$$

The boundary conditions are

$$\psi_{1/2,m} = \psi_{1/2,m^*}, 0 < \mu_m \le 1, m^* : \mu_{m^*} = -\mu_m, \quad (13)$$

$$\psi_{N_x+1/2,m} = \psi_m^{in}, 1 \le \mu_m < 0, \psi_m^{in} = \psi^{in}(\mu_m). \quad (14)$$

Here $\psi_{m,i}$ is the cell-midpoint angular flux, and $\psi_{m,i+1/2}$ is the cell-edge one. The subscripts L and R denote functions

spatially averaged over the left- and right-half of the i-th cell, respectively:

$$\psi_{L,m,i} = \frac{2}{h_i}\int_{x_{i-1/2}}^{x_i} \psi(x,\mu_m)\,dx,$$
$$\psi_{R,m,i} = \frac{2}{h_i}\int_{x_i}^{x_{i+1/2}} \psi(x,\mu_m)\,dx. \tag{15}$$

The scalar flux in the right sides of the difference equations (8)–(11) is approximated in the i-th cell by the exponential:

$$\tilde{\phi}_i(x) = \alpha_i e^{\beta_i(x-x_i)},\ x_{i-1/2} < x < x_{i+1/2}. \tag{16}$$

The interpolation parameters α_i and β_i are determined by the conditions:

$$\frac{2}{h_i}\int_{x_{i-1/2}}^{x_i} \alpha_i e^{\beta_i(x-x_i)}\,dx = \phi_{L,i}, \tag{17}$$

$$\frac{2}{h_i}\int_{x_i}^{x_{i+1/2}} \alpha_i e^{\beta_i(x-x_i)}\,dx = \phi_{R,i}. \tag{18}$$

The use of this approximation gives rise to the nonlinearity of the difference scheme. Solving Eqs. (17) and (18) for α_i and β_i, we have

$$\alpha_i = \frac{\phi_{R,i}\phi_{L,i}}{\phi_{R,i}-\phi_{L,i}}\log\left(\frac{\phi_{R,i}}{\phi_{L,i}}\right), \tag{19}$$

$$\beta_i = \frac{2}{h_i}\log\left(\frac{\phi_{R,i}}{\phi_{L,i}}\right). \tag{20}$$

Then, using Eqs. (8)–(11), (19) and (20), we obtain the following nonlinear difference characteristic (NDC) equations:

$$\psi_{m,i} = \psi_{m,i+1/2}e^{-\tau_{m,i}} + \frac{Q_i}{2\sigma_{t,i}}(1-e^{-\tau_{m,i}}) + \frac{1}{4\mu_m}\sigma_{s,i}\phi_{R,i}\theta^-_{m,i}, \tag{21}$$

$$\psi_{m,i-1/2} = \psi_{m,i}e^{-\tau_{m,i}} + \frac{Q_i}{2\sigma_{t,i}}(1-e^{-\tau_{m,i}}) + \frac{1}{4\mu_m}\sigma_{s,i}\phi_{L,i}\theta^-_{m,i}, \tag{22}$$

$$i = 1, ..., N_x,\ -1 \le \mu_m < 0,$$

$$\psi_{m,i} = \psi_{m,i-1/2}e^{-\tau_{m,i}} + \frac{Q_i}{2\sigma_{t,i}}(1-e^{-\tau_{m,i}}) + \frac{1}{4\mu_m}\sigma_{s,i}\phi_{L,i}\theta^+_{m,i}, \tag{23}$$

$$\psi_{m,i+1/2} = \psi_{m,i}e^{-\tau_{m,i}} + \frac{Q_i}{2\sigma_{t,i}}(1-e^{-\tau_{m,i}}) + \frac{1}{4\mu_m}\sigma_{s,i}\phi_{R,i}\theta^+_{m,i}, \tag{24}$$

$$i = 1, ..., N_x,\ -1 \le \mu_m < 1,$$

where

$$\tau_{m,i} = \frac{\sigma_{t,i}h_i}{2|\mu_m|}, \tag{25}$$

$$\theta^-_{m,i} = \theta_{m,i}(z_i), \tag{26}$$

$$\theta^+_{m,i} = -\theta_{m,i}\left(\frac{1}{z_i}\right), \tag{27}$$

$$\theta_{m,i}(y) = \frac{(1-ye^{-\tau_{m,i}})h_i\log y}{(\log y-\tau_{m,i})(y-1)}, \tag{28}$$

$$z_i = \frac{\phi_{R,i}}{\phi_{L,i}}. \tag{29}$$

The NLCB method for the transport equation (1)–(2) is defined by the two HCB equations (5)–(6) and four NDC equations (21)–(24), which contain nonlinear scattering-like terms. Our proposed method for solving NLCB equations consists of iterations that cope with the nonlinearity of the scheme and with the scattering.

3. ACCELERATION METHOD

The proposed method for solving the nonlinear NLCB method (5), (6) and (21)–(29) with boundary conditions (13) and (14) is based on the nonlinear averaged flux (AF) method [9, 10]. To derive this method, the transport equation is integrated over $-1 \le \mu \le 0$ and over $0 \le \mu \le 1$. To close the resulting set of equations, special functionals are introduced. One obtains:

$$\mu\frac{\partial}{\partial x}\psi(x,\mu) + \sigma_t(x)\psi(x,\mu) = \frac{1}{2}(\sigma_s(x)\phi(x) + Q(x)), \tag{30}$$

$$\psi(0,\mu) = \psi(0,-\mu),\ 0 < \mu \le 1, \tag{31}$$

$$\psi(L,\mu) = \psi^{in}(\mu),\ -1 \le \mu < 0, \tag{32}$$

$$G^-(x) = \int_{-1}^{0}\mu\psi(x,\mu)\,d\mu \Big/ \int_{-1}^{0}\psi(x,\mu)\,d\mu, \tag{33}$$

$$G^+(x) = \int_{0}^{1}\mu\psi(x,\mu)\,d\mu \Big/ \int_{0}^{1}\psi(x,\mu)\,d\mu, \tag{34}$$

$$\frac{d}{dx}\left(G^{-}(x)\phi^{-}(x)\right)+\left(\sigma_t(x)-\frac{1}{2}\sigma_s(x)\right)\phi^{-}(x)$$
$$=\frac{1}{2}\left(\sigma_s(x)\phi^{+}(x)+Q(x)\right), \tag{35}$$

$$\frac{d}{dx}\left(G^{+}(x)\phi^{+}(x)\right)+\left(\sigma_t(x)-\frac{1}{2}\sigma_s(x)\right)\phi^{+}(x)$$
$$=\frac{1}{2}\left(\sigma_s(x)\phi^{-}(x)+Q(x)\right), \tag{36}$$

$$\phi^{+}(0)=\phi^{-}(0), \tag{37}$$

$$\phi^{-}(L)=\phi^{in}, \tag{38}$$

$$\phi(x)=\phi^{+}(x)+\phi^{-}(x). \tag{39}$$

Here

$$\phi^{-}(x)=\int_{-1}^{0}\psi(x,\mu)\,d\mu,\ \phi^{+}(x)=\int_{0}^{1}\psi(x,\mu)\,d\mu \tag{40}$$

are the partial scalar fluxes, and

$$\phi^{in}=\int_{-1}^{0}\psi^{in}(\mu)\,d\mu. \tag{41}$$

We note that the resulting nonlinear problem (30)–(39) is equivalent to the original linear transport problem (1)–(4).

The nonlinear system of equations (30)–(39) is solved iteratively, with three steps per iteration:

1. Assuming that the functionals $G^{\pm(k)}$ are known from the previous (k-th) outer iteration, the low-order transport problem [Eqs. (35)–(38)] is solved for the partial scalar fluxes $\phi^{\pm(k+1)}(x)$ to obtain the scalar flux

$$\frac{d}{dx}G^{\pm(k)}\phi^{\pm(k+1)}+\left(\sigma_t-\frac{1}{2}\sigma_s\right)\phi^{\pm(k+1)}=\frac{1}{2}\left(\sigma_s\phi^{\mp(k+1)}+Q\right), \tag{42}$$

$$\phi^{+(k+1)}(0)=\phi^{-(k+1)}(0), \tag{43}$$

$$\phi^{-(k+1)}(L)=\phi^{in}, \tag{44}$$

$$\phi^{(k+1)}=\phi^{+(k+1)}+\phi^{-(k+1)}. \tag{45}$$

2. Using the scalar flux $\phi^{(k+1)}(x)$ from step 1, we solve the following transport problem to determine $\psi^{(k+1)}(x,\mu)$:

$$\mu\frac{\partial\psi^{(k+1)}}{\partial x}+\sigma_t\psi^{(k+1)}=\frac{1}{2}\left(\sigma_s\phi^{(k+1)}+Q\right), \tag{46}$$

$$\psi^{(k+1)}(0,\mu)=\psi^{(k+1)}(0,-\mu),\ 0<\mu\le 1, \tag{47}$$

$$\psi^{(k+1)}(L,\mu)=\psi^{in}(\mu),\ -1\le\mu<0. \tag{48}$$

3. Using the new angular flux $\psi^{(k+1)}(x,\mu)$ from step 2, we calculate the functionals $G^{\pm(k+1)}(x)$ [Eqs. (33)–(34)]:

$$G^{\pm(k+1)}=\int_{0}^{\pm1}\mu\psi^{(k+1)}\,d\mu\Big/\int_{0}^{\pm1}\psi^{(k+1)}\,d\mu. \tag{49}$$

For the first iteration ($k=0$) the functionals $G^{\pm(0)}$ are calculated by assuming an isotropic angular flux $\psi^{(0)}(x,\mu)$.

The AF method is stable for independent discretizations of the high-order and low-order transport problems. However, to develop a pure acceleration method for the NLCB method, based on the AF method, we use a consistent difference scheme. To derive the discretization of the low-order equations (35)–(36) consistent with the NLCB scheme, we first sum the HCB equations (5) and (6) in a way that corresponds to the integrations over $-1\le\mu$ and $0\le\mu\le1$. We use a quadrature set $\{\mu_m, w_m\}$ that satisfies the conditions:

$$\sum_{m\in M^{\pm}}w_m=1, \tag{50}$$

where

$$M^{-}=\{m:\mu_m\le0\},\ M^{+}=\{m:\mu_m\ge0\}. \tag{51}$$

Thus, we sum the NDC equations (21)–(24) over $M^{\pm}$ in each half-cell with weight μ_m. To close the resulting difference equations, we introduce functionals similar to $G^{\pm}(x)$ [Eqs. (33)–(34)]:

$$G^{\pm}_{i}=\sum_{m\in M^{\pm}}\mu_m\psi_{m,i}w_m\Big/\sum_{m\in M^{\pm}}\psi_{m,i}w_m, \tag{52}$$

$$G^{\pm}_{i-1/2}=\sum_{m\in M^{\pm}}\mu_m\psi_{m,i-1/2}w_m\Big/\sum_{m\in M^{\pm}}\psi_{m,i-1/2}w_m, \tag{53}$$

$$F^{\pm}_{i}=\sum_{m\in M^{\pm}}\mu_m e^{-\tau_{m,i}}\psi_{m,i}w_m\Big/\sum_{m\in M^{\pm}}\mu_m\psi_{m,i}w_m, \tag{54}$$

$$F^{\pm}_{i\mp1/2}=\sum_{m\in M^{\pm}}\mu_m e^{-\tau_{m,i}}\psi_{m,i\mp1/2}w_m\Big/\sum_{m\in M^{\pm}}\mu_m\psi_{m,i\mp1/2}w_m, \tag{55}$$

$$E^{\pm}_{i}=\sum_{m\in M^{\pm}}\mu_m(1-e^{-\tau_{m,i}})w_m, \tag{56}$$

$$P^{\pm}_{i}=\sum_{m\in M^{\pm}}\theta^{\pm}_{m,i}w_m, \tag{57}$$

$$i=1,\ldots,N_x.$$

The discrete low-order problem of the AF method consistent with the NLCB scheme then has the following form:

$$G_i^{\pm}\phi_i^{\pm} - G_{i-1/2}^{\pm}\phi_{i-1/2}^{\pm} + \frac{1}{2}\left(\sigma_{t,i} - \frac{1}{2}\sigma_{s,i}\right)h_i\phi_{L,i}^{\pm} = \frac{1}{4}h_i(\sigma_{s,i}\phi_{L,i}^{\mp} + Q_i), \tag{58}$$

$$G_{i+1/2}^{\pm}\phi_{i+1/2}^{\pm} - G_i^{\pm}\phi_i^{\pm} + \frac{1}{2}\left(\sigma_{t,i} - \frac{1}{2}\sigma_{s,i}\right)h_i\phi_{R,i}^{\pm} = \frac{1}{4}h_i(\sigma_{s,i}\phi_{R,i}^{\mp} + Q_i), \tag{59}$$

$$G_i^{-}\phi_i^{-} = G_{i+1/2}^{-}\phi_{i+1/2}^{-} + \frac{Q_i}{2\sigma_{t,i}}E_i^{-} + \frac{1}{4}\sigma_{s,i}\phi_{R,i}P_i^{-}, \tag{60}$$

$$G_{i-1/2}^{-}\phi_{i-1/2}^{-} = G_i^{-}\phi_i^{-} + \frac{Q_i}{2\sigma_{t,i}}E_i^{-} + \frac{1}{4}\sigma_{s,i}\phi_{L,i}P_i^{-}, \tag{61}$$

$$G_i^{+}\phi_i^{+} = G_{i-1/2}^{+}\phi_{i-1/2}^{+} + \frac{Q_i}{2\sigma_{t,i}}E_i^{+} + \frac{1}{4}\sigma_{s,i}\phi_{L,i}P_i^{+}, \tag{62}$$

$$G_{i+1/2}^{+}\phi_{i+1/2}^{+} = G_i^{+}\phi_i^{+} + \frac{Q_i}{2\sigma_{t,i}}E_i^{+} + \frac{1}{4}\sigma_{s,i}\phi_{R,i}P_i^{+}, \tag{63}$$

where

$$\phi_i^{\pm} = \sum_{m\in M^{\pm}}\psi_{m,i}w_m, \tag{64}$$

$$\phi_{i-1/2}^{\pm} = \sum_{m\in M^{\pm}}\psi_{m,i-1/2}w_m, \tag{65}$$

$$\phi_{L,i}^{\pm} = \sum_{m\in M^{\pm}}\psi_{L,m,i}w_m, \tag{66}$$

$$\phi_{R,i}^{\pm} = \sum_{m\in M^{\pm}}\psi_{R,m,i}w_m, \tag{67}$$

$$\phi_{R,i} = \phi_{R,i}^{-} + \phi_{R,i}^{+}, \tag{68}$$

$$\phi_{L,i} = \phi_{L,i}^{-} + \phi_{L,i}^{+}. \tag{69}$$

To derive boundary conditions for the low-order problems, we sum the boundary conditions (13) and (14) for the transport differencing equations by means of the quadrature set $\{\mu_m, w_m\}$ to get

$$\phi_{1/2}^{+} = \phi_{1/2}^{-}, \tag{70}$$

$$\phi_{N_x+1/2}^{-} = \hat{\phi}^{in}, \tag{71}$$

where

$$\hat{\phi}^{in} = \sum_{m\in M^{-}}\psi_m^{in}w_m.$$

The complete set of difference equations of the nonlinear AF method for the NLCB method consists of the high-order transport problem (5), (6), (13), (14), and (21)–(24), the set of functionals (52)–(57), and the low-order problem (58)–(63), (70), and (71). This system of equations is solved according to a nonlinear iteration procedure that is similar to the one described above [Eqs. (42)–(49)]. If some guess for the scalar flux is known, then one can calculate the angular flux from the transport differencing equations (5), (6), (13), (14), and (21)–(24), in spite of the fact that the right-hand sides of the NDC equations (21)–(24) are nonlinear with respect to the scalar flux. However, to solve the nonlinear low-order problem for the partial scalar fluxes, we linearize Eqs. (60)–(63) with respect to $\phi_{L,i}$ and $\phi_{R,i}$ by means of Newton's method. These equations contain nonlinear terms $\phi_{R,i}P_i^{\pm}$ and $\phi_{L,i}P_i^{\pm}$, where $P_i^{\pm} = P^{\pm}(z_i)$, $z_i = \phi_{R,i}/\phi_{L,i}$ (see Eqs. (26)–(29) and (57)). On the s-th Newton's iteration, these terms have the form:

$$\phi_{R,i}^{(s)}P_i^{\pm(s)} = \phi_{R,i}^{(s-1)}P_i^{\pm(s-1)} + \left(\frac{\partial\phi_R P^{\pm}}{\partial\phi_R}\right)_i^{(s-1)}(\phi_{R,i}^{(s)} - \phi_{R,i}^{(s-1)}) + \left(\frac{\partial\phi_R P^{\pm}}{\partial\phi_L}\right)_i^{(s-1)}(\phi_{L,i}^{(s)} - \phi_{L,i}^{(s-1)}), \tag{72}$$

$$\phi_{L,i}^{(s)}P_i^{\pm(s)} = \phi_{L,i}^{(s-1)}P_i^{\pm(s-1)} + \left(\frac{\partial\phi_L P^{\pm}}{\partial\phi_R}\right)_i^{(s-1)}(\phi_{R,i}^{(s)} - \phi_{R,i}^{(s-1)}) + \left(\frac{\partial\phi_L P^{\pm}}{\partial\phi_L}\right)_i^{(s-1)}(\phi_{L,i}^{(s)} - \phi_{L,i}^{(s-1)}). \tag{73}$$

Rearrangement of Eqs. (72) and (73) gives

$$\phi_{R,i}^{(s)}P_i^{\pm(s)} = \left(P_i^{\pm(s-1)} + z_i^{(s-1)}\left(\frac{\partial P^{\pm}}{\partial z}\right)_i^{(s-1)}\right)\phi_{R,i}^{(s)} - (z_i^{(s-1)})^2\left(\frac{\partial P^{\pm}}{\partial z}\right)_i^{(s-1)}\phi_{L,i}^{(s)}, \tag{74}$$

$$\phi_{L,i}^{(s)}P_i^{\pm(s)} = \left(P_i^{\pm(s-1)} - z_i^{(s-1)}\left(\frac{\partial P^{\pm}}{\partial z}\right)_i^{(s-1)}\right)\phi_{L,i}^{(s)} + \left(\frac{\partial P^{\pm}}{\partial z}\right)_i^{(s-1)}\phi_{R,i}^{(s)}. \tag{75}$$

We note that in one-dimensional geometry, the linearized low-order difference problem can be solved directly as in the case with other methods such as QD or DSA. In one-dimensional geometries various methods are nearly equal from the viewpoint of computations required for solving the low-order problem. However, in multi-dimensional geometries it will be necessary to develop efficient iterative methods for solving low-order equations of the AF method, for example, using the transport synthetic acceleration method [20].

Finally, we have the iteration procedure (*outer iterations*), which consists of the following three steps:

TABLE I

Number of Iterations versus N_x for Problem 1

		NLCB method with AF method			
N_x	$\sigma_t h$	Number of outer iterations	Total number of inner iterations	SI method	NLC method: Total number of DSA iterations
2	30.0	3	12	812	19
4	15.0	3	11	547	17
8	7.5	4	12	462	17
16	3.25	5	14	446	17
32	1.875	5	13	444	18
64	0.9375	6	15	444	20
128	0.46875	7	16	444	20

1. Assuming that functionals $G_{\bar{i}}^{\pm(k)}$, $G_{\bar{i}-1/2}^{\pm(k)}$, $F_{\bar{i}}^{\pm(k)}$, $F_{\bar{i}\mp1/2}^{\pm(k)}$, [Eqs. (52)–(55)] are known, we solve the linearized low-order problem [Eqs. (58)–(63), (68)–(71), (74), and (75)] by Newton's method to obtain partial scalar fluxes $\phi_{\bar{i}}^{\pm(k+1)}$, $\phi_{\bar{i}-1/2}^{\pm(k+1)}$, $\phi_{L,i}^{\pm(k+1)}$, and $\phi_{R,i}^{\pm(k+1)}$ (*inner iterations*). Then, we calculate the scalar fluxes $\phi_{L,i}^{(k+1)}$ and $\phi_{R,i}^{(k+1)}$.

2. Using the scalar fluxes obtained from the low-order problem, we solve the NLCB equations [Eqs. (5), (6), (13), (14), and (21)–(29)] to determine the angular fluxes $\psi_{m,i}^{(k+1)}$, $\psi_{m,i-1/2}^{(k+1)}$, $\psi_{L,m,i}^{(k+1)}$ and $\psi_{R,m,i}^{(k+1)}$.

3. Using $\psi_i^{(k+1)}$ and $\psi_{i-1/2}^{(k+1)}$, we calculate the functionals $G_{\bar{i}}^{\pm(k+1)}$, $G_{\bar{i}-1/2}^{\pm(k+1)}$, $F_{\bar{i}}^{\pm(k+1)}$, and $F_{\bar{i}\mp1/2}^{\pm(k+1)}$ [Eqs. (52)–(55)].

The functionals $E_{\bar{i}}^{\pm}$ [Eq. (56)] do not change during iterations, so they may be precalculated. For the first outer iteration ($k = 0$), we calculate the functionals $G_{\bar{i}}^{\pm(0)}$, $G_{\bar{i}-1/2}^{\pm(0)}$, $F_{\bar{i}}^{\pm(0)}$, $F_{\bar{i}\mp1/2}^{\pm(0)}$ by assuming that the angular flux $\psi^{(0)}$ is isotropic. As an initial guess for the inner (Newton's) iterations, we use the solution of the low-order problem from the previous outer iteration.

The converged solution of each low-order problem is strictly positive. However, the solution of the linearized low-order problem during a given Newton's iteration may be nonpositive in some spatial mesh cells. The linearized discrete low-order equations contain terms with $\log z_i$, where $z_i = \phi_{R,i}/\phi_{L,i}$. Hence, it is impossible to proceed with inner iterations if $z_i \le 0$, and we need to fix up nonpositive values of z_i. If $z_i^{(s)} = z^*$, $z^* \le 0$ for some $i = i^*$, then in this mesh cell we change the value $z_{i^*}^{(s)}$ to $\frac{1}{2}(z_{i^*}^{(s-1)} + z^*)$. We repeat this procedure until $z_{i^*}^{(s)}$ becomes positive. We have not experienced any difficulties with this simple algorithm.

TABLE II

Numbers of Inner Iterations for Problem 1

	Outer iteration						
N_x	1	2	3	4	5	6	7
2	8	2	2	—	—	—	—
4	7	2	2	—	—	—	—
8	6	2	2	2	—	—	—
16	5	3	2	2	2	—	—
32	4	3	2	2	2	—	—
64	5	2	2	2	2	2	—
128	4	2	2	2	2	2	2

An iterative algorithm for the NLCB method similar to that described above can also be developed by means of nonlinear α-weighted acceleration (α-WA) methods [16]. This parametrized family of nonlinear acceleration methods is a generalization of the nonlinear "flux" methods. The low-order problems of α-WA methods are obtained by integrating the transport equation over $-1 \le \mu \le 0$ and $0 \le \mu \le 1$ with weights $|\mu|^\alpha$, where the constant $\alpha \ge 0$. To close this system of equations, functionals similar to $G^{\pm}$ are introduced. The nonlinear α-WA methods with $\alpha = 0$ and $\alpha = 1$ correspond to the AF (or first-flux) and second-flux [15] methods, respectively. Methods with particular values of the parameter α have certain advantages compared to others. For example, the consideration of these methods in differential form shows that the method with $\alpha = 0.128$ possesses a minimum spectral radius for the scattering ratio $c = 1$.

We considered the α-WA family of iteration methods for the consistently-differenced NLCB scheme. We found that the choice $\alpha = 0$ (namely, the AF method) gives the best acceleration of the NLCB scheme in most problems. The method with $\alpha = 0.128$ converges slightly faster than the AF method only for $c \approx 1$ and optically thin mesh cells.

4. NUMERICAL RESULTS

To demonstrate the efficiency of the proposed acceleration method, we present numerical results from three test problems.

TABLE III

$\Delta^{(k)}$ for Problem 1

	Outer iteration (k)				
N_x	3	4	5	6	7
2	1.2×10^{-7}	—	—	—	—
4	9.0×10^{-6}	—	—	—	—
8	5.3×10^{-4}	1.4×10^{-3}	—	—	—
16	6.6×10^{-3}	1.2×10^{-2}	1.3×10^{-2}	—	—
32	3.6×10^{-2}	$3{,}1 \times 10^{-2}$	3.2×10^{-2}	—	—
64	8.6×10^{-2}	4.6×10^{-2}	4.2×10^{-2}	5.0×10^{-2}	—
128	7.6×10^{-2}	6.0×10^{-2}	7.8×10^{-2}	7.2×10^{-2}	9.9×10^{-2}

Problem 1: This is a homogeneous slab $0 \le x \le 60$ cm, with $\sigma_t = 1$ cm^{-1}, $\sigma_s = 0.95$ cm^{-1}, and $Q = 0$. The left boundary has an isotropic incident flux with magnitude unity, and the right boundary has no incident flux [18]. We use the standard S_{16} Gauss-Legendre quadrature set and uniform spatial grids. The relative pointwise convergence criteria are $\varepsilon_{inner} = 10^{-5}$ (for inner iterations) and $\varepsilon_{outer} = 10^{-4}$ (for outer iterations). In solving the problems by the SI method, we use the convergence criterion in the following form:

$$\max_{i\in[1,N_x+1]} \left| 1 - \frac{\phi_{i-1/2}^{(k)}}{\phi_{i-1/2}^{(k)}} \right| \le (1-\rho)\,\varepsilon_{outer}, \tag{76}$$

where ρ is the spectral radius, numerically estimated in L_2-norm. This protects from false convergence.

In Table 1 we list the number of iterations for the NLCB scheme, solved by the new acceleration method and by the SI method. The results are obtained for various numbers of spatial mesh cells N_x. Table 1 also shows the results for the nonlinear characteristic (NLC) method [18] accelerated by the DSA method. Wareing *et al.* [18] first linearized the NLC method with respect to certain parameters. Then, the resulting linear transport problem was solved by means of the DSA method. The total numbers of the DSA linear transport iterations in this problem are presented. In Table 2, the distribution of numbers of inner iterations during outer iterations is shown. In Table 3, we listed the values

$$\Delta^{(k)} = \frac{\max_i |\phi_i^{(k)} - \phi_i^{(k-1)}|}{\max_i |\phi_i^{(k-1)} - \phi_i^{(k-2)}|}, 1 \le i \le N_x, \tag{77}$$

which characterize the rate of error decrease during the outer iterations. To show the accuracy of the calculations by means of the NLCB methods in deep penetration problems and compare the results with the NLC method [18] and DD method [19], in Table 4 we present the values of the outgoing current on the right boundary ($x = L$)

$$I^+(L) = \int_0^1 \mu\psi(L,\mu)\,d\mu$$

for various N_x.

TABLE IV

$I^+(L)$ for Problem 1

N_x	NLCB	NLC	DD
2	6.33×10^{-11}	5.68×10^{-11}	1.77×10^{-1}
4	5.43×10^{-11}	5.56×10^{-11}	2.05×10^{-2}
8	4.55×10^{-11}	4.67×10^{-11}	1.14×10^{-3}
16	4.19×10^{-11}	4.20×10^{-11}	1.34×10^{-4}
32	4.10×10^{-11}	4.09×10^{-11}	5.90×10^{-5}
64	4.07×10^{-11}	4.07×10^{-11}	3.18×10^{-11}
128	4.07×10^{-11}	4.07×10^{-11}	3.83×10^{-11}

These results illustrate several key points. First, the new iteration scheme is extremely effective at reducing the number of high-order transport sweeps, compared to both SI and to the DSA algorithm for the NLC method [18] of Wareing *et al.* The number of high-order sweeps in the new scheme varied from 3 to 7; with SI, the range was 444 to 812; and with the DSA algorithm for the NLC method [18] the range was 17 to 20. This reduction in the number of high-order sweeps results from our strategy of doing as much work as possible in the low-order equations. Second, inner (Newton's) iterations converged quickly, never taking more than 7 iterations for a low-order problem and never totaling more than 16 for all low-order solutions in one overall problem. We ran this problem on a Sun SPARCstation 10 model Q90 with the operating system Solaris 2.5.1. For $N_x = 64$, 3.1 seconds were required for the SI method and 0.3 seconds for the new method. [We measured only the time spent in the execution of commands (user time).] The execution time of one Newton's iteration in the low-order problem is about 2.5 times as great as the time for the transport sweep in the high-order problem. However, the efficient acceleration gives rise to significantly reduced execution time as a whole. Note that

TABLE V

Parameters of Problem 2

Region number	1	2	3
Right boundary (cm)	25	40	100
σ_t (cm$^{-1)}$	1.0	1.0	1.0
σ_s (cm^{-1})	0.8	0.99	0.7
Q (cm^{-3} s^{-1})	0.1	1.0	0.05

TABLE VI

Number of Iterations versus N_x for Problem 2

N_x	Number of cells in region			NLCB method with AF method		SI method	NLC method: Total number of DSA iterations
	1	2	3	Number of outer iterations	Total number of inner iterations		
4	1	1	2	3	10	242	8
8	2	2	4	3	9	416	10
16	4	4	8	4	11	447	12
32	8	8	16	4	12	451	10
64	16	16	32	5	13	452	7
128	32	32	64	5	14	452	7

we did not optimize the method for solving the matrix system in the low-order problem. We simply used banded solver from LAPACK[21]. In multidimensional problems, however, it will be essential to devise an efficient solution procedure for the low-order system, for the cost of direct inversion will be prohibitive in many cases. The low-order solution will require considerable care in multidimensional geometries because in this case the computational cost of the low-order problem is much greater, in a relative sense compared to the high-order problem.

Problem 2: This problem is a slab $0 \le x \le 100$ cm with vacuum boundaries [18]. The slab consists of three regions, whose parameters are listed in Table 5. The spatial cells in each region are uniform. The S_{16} Gauss-Legendre quadrature set was used. The relative pointwise convergence criteria are $\varepsilon_{inner} = 10^{-5}$ and $\varepsilon_{outer} = 10^{-4}$.

The results of calculations by means of the new and the SI method are presented in Table 6. This table shows also the numerical results of the NLC scheme accelerated by the DSA method [18]. In Table 7 we show the number of inner (Newton's) iterations for each outer iteration. The values of $\Delta^{(k)}$ [Eq. (77)] are listed in Table 8.

In this multiregion problem, the number of high-order sweeps in the new method varied from 3 to 5, while in case of the SI method the range was 242 to 452. The number of linear transport iterations of the NLC method with the DSA algorithm [18] ranged from 7 to 12. The total number of inner (Newton's) iterations in the low-order problem for the new method varied from 9 to 14. This problem for $N_x = 64$ required 3.3 seconds for the SI method and 0.3 seconds for the new method. These results show again that the proposed method efficiently accelerates the iterative convergence of the NLCB scheme.

TABLE VII

Numbers of Inner Iterations for Problem 2

N_x	Outer iteration				
	1	2	3	4	5
4	6	2	2	—	—
8	5	2	2	—	—
16	5	2	2	2	—
32	5	3	2	2	—
64	4	3	2	2	2
128	5	3	2	2	2

In Problem 1 for $N_x = 64$ and 128, and in Problem 2 for $N_x = 4$ and 128, $z_i = \phi_{R,i}/\phi_{L,i}$ becomes nonpositive in some spatial cells during the inner (Newton's) iterations, and the fixup procedure described above was used. All these cases of $z_i < 0$ occur on the first outer iteration during either the first or second Newton's (inner) iterations, i.e. at the very beginning of the whole iteration process. The reason for the nonpositivity of z_i is an inaccurate initial guess. Note that the number of iterations in these cases did not change compared to results for other spatial meshes in which z_i in the low-order problem during the inner iterations is always positive. We conclude from this and other tests that our simple z fixup does not degrade the convergence of the Newton's iterations.

Problem 3: This is a homogeneous slab $0 \le x \le 60$ cm, with vacuum boundaries, $\sigma_t = 1$ cm^{-1}, $\sigma_s = 1$ cm^{-1}, and $Q = 1$ cm^{-3} s^{-1} [17]. The standard S_{16} Gauss-Legendre quadrature set and uniform spatial grids are utilized. The relative pointwise convergence criteria are $\varepsilon_{inner} = 10^{-5}$ and $\varepsilon_{outer} = 10^{-4}$.

Table 9 presents the results for various numbers of mesh cells N_x. In this table we show the number of outer iterations in the proposed algorithm for the NLCB method provided the Newton's (inner) iterations in the low-order problem are converged. The total number of Newton's (inner) iterations is shown in parentheses. The results of the NLC scheme accelerated by the AF method [17] are also listed. This algorithm for the NLC scheme is equivalent to only one Newton's iteration in each low-order problem. In most cases the number of transport sweeps in this method is two times greater than in the presented iteration

TABLE VIII

$\Delta^{(k)}$ for Problem 2

	Outer iteration (k)		
N_x	3	4	5
4	1.7×10^{-8}	—	—
8	1.1×10^{-3}	—	—
16	1.3×10^{-2}	1.3×10^{-2}	—
32	2.2×10^{-2}	2.5×10^{-2}	—
64	2.7×10^{-2}	2.1×10^{-2}	5.3×10^{-2}
128	3.6×10^{-2}	2.5×10^{-2}	5.9×10^{-2}

algorithm for the NLCB method. We also performed calculations with only one Newton's (inner) iteration in the low-order problem, and included our results. They are similar to the results of the acceleration algorithm for the NLC method based on the AF method [17]. Thus, if one performs Newton's iterations in the low-order problem until convergence, one obtains in significant reduction in the number of outer iterations, i.e. transport sweeps.

The results of these three test problems show that the new acceleration method for the NLCB method converges much more rapidly than source iteration. Also, the number of Newton's (inner) iterations in each low-order problem is small. Because the NLCB method and the NLC method have similar nonlinearities, it is interesting to compare the efficiency of various approaches for accelerating these two methods. In most of the test problems presented above, the number of outer iterations (transport sweeps) required by the new method for the NLCB scheme is at most half the number of high-order transport sweeps required by iteration algorithms for the NLC scheme based on the AF and DSA methods [17, 18]. This means that in the new acceleration method the high-order problem is solved noticeably fewer times compared to the method [17, 18] presented by Wareing *et al.* The main difference in the presented method from the acceleration method in [18] is that Newton's linearization is performed in the inexpensive low-order problem. The new method differs from the acceleration method in [17], which also uses the linearized low-order problem generated by means of the AF method, in that the linearized low-order problem is solved by Newton's iterations until convergence. Thus, most of the acceleration work in the developed method is done on the low-order level. Also, the fixup of a negative transport iterate in the low-order problem does not influence the number of outer iterations because the converged low-order scalar flux is always positive.

5. DISCUSSION

We have developed a rapidly convergent iteration algorithm, based on the AF method, for the NLCB scheme. The linearization of this nonlinear spatial difference scheme is performed in the low-order problem, resulting in considerable computational savings. The Newton's iterations are performed until convergence. The number of Newton's iterations on the low-order problem is small.

In multi-dimensional geometries it is necessary to develop efficient iterative methods for solving low-order equations of the AF method. Note that other nonlinear iteration methods, such as the quasi-diffusion method [14], can also be used in place of AF in our iteration framework. For multi-dimensional problems, one should choose the basic method that generates the low-order problem that is easiest to solve. These are subjects of future research. Finally, we note that the algorithm described here can be applied to other nonlinear transport differencing schemes.

TABLE IX

Number of Iterations versus N_x for Problem 3

		NLCB method with AF method: Number of outer iterations		
N_x	$\sigma_t h$	With converged Newton's (inner) iterations	With one Newton's (inner) iteration	NLC method with AF method
2	30.	3 (10)[a]	6	6
3	20.	3 (10)	6	6
4	15	3 (10)	6	6
6	10	3 (10)	6	6
12	5	4 (11)	6	6
30	3	4 (11)	8	5
60	1	4 (10)	6	4
600	0.1	5 (12)	12	12

[a] The values in parentheses are the total number of Newton's (inner) iterations.

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