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A STABLE SHIFTED-LEGENDRE PROJECTION SCHEME FOR GENERATING P_N BOUNDARY CONDITIONS

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Abstract—A projection scheme for generating P_N boundary conditions based on the shifted Legendre polynomials is discussed. The projection scheme yields $N+1$ conditions for each boundary of a slab, just twice the number of conditions required. The resulting overdetermined system of equations is subsequently reduced to a square system by means of a standard least-squares technique. Tests carried out for several problems indicate that the procedure is numerically stable in high-order, in contrast to the findings of some years ago when a similar projection scheme was first proposed.

1. INTRODUCTION

As is well known (Davison, 1957; Gelbard, 1968), the spherical-harmonics (P_N) method for solving transport problems cannot accommodate boundary conditions exactly, and so this aspect of the method has become a subject of research interest in transport theory. In the 40's, Marshak (1947) and Mark (1945) developed the boundary conditions that carry their names and that are still widely used (Garcia *et al.*, 1994a). In the 60's, Federighi (1964) and Pomraning (1964a, 1964b) introduced the idea of using variational principles to derive boundary conditions for the P_N method. Recently, Larsen and Pomraning (1991) derived a class of P_N boundary conditions by means of asymptotic analysis. A comparison of the performance of all these types of boundary conditions in low order ($N \leq 5$) has been reported (Rulko *et al.*, 1991), the main conclusion being that there is no boundary condition that can be identified as the most (or the least) accurate for all problems.

Some years ago we used (Garcia and Siewert, 1982) a projection scheme based on the polynomials $\mu P_k(2\mu-1)$, where $P_k(2\mu-1)$ denote the shifted Legendre polynomials, to generate the boundary conditions required in a spherical-harmonics solution of the standard problem in radiative transfer (Chandrasekhar, 1950). Since in transport problems boundary conditions are always specified on an half-range interval for the μ variable—(0,1) or its negative counterpart—and the shifted Legendre polynomials are half-range orthogonal, it was expected that such a scheme could be an improvement over the traditional Marshak scheme. Although the shifted Legendre scheme did, in fact, prove to be more accurate than the Marshak scheme for the considered test problem (Garcia and Siewert, 1982), later on it yielded ill-conditioned linear systems when used in high order for a more challenging class of problems (Benassi *et al.*, 1984), and since then it has not been used again.

In this paper we reexamine the idea of using the shifted Legendre polynomials to define a projection scheme for generating P_N boundary conditions for azimuthally symmetric problems. However, instead of using the polynomials $\mu P_k(2\mu - 1)$ for $k = 0, 1, \ldots, (N - 1)/2$ as in our previous work (Garcia and Siewert, 1982), we use the polynomials $P_k(2\mu - 1)$, $k = 0, 1, \ldots, N$, to define our projection scheme. Our motivation for this choice comes from the fact that moments of order $> N$ do not make any additional contribution when this projection scheme is used, provided one can express the original boundary conditions of the problem as polynomials of degree no larger than N. In this way, we find exactly twice the number of conditions we require, and so we use least-squares (Jennings, 1977) to reduce the resulting overdetermined system of equations to a square system for the coefficients of the P_N approximation. Unlike the procedure of our previous work (Garcia and Siewert, 1982), our new procedure yielded well-conditioned systems in high order for all test problems that we tried.

The outline of the paper is as follows. In Sec. 2, we report our proposed projection scheme to obtain P_N boundary conditions and the least-squares technique that we use for reducing the overdetermined system to a square system. In Sec. 3, we discuss some aspects relevant to the computational implementation of our procedure. In Sec. 4, we record some observations regarding the performance of our projection scheme as compared to the Mark and Marshak schemes, and we tabulate some numerical results for a test problem. Finally, in Sec. 5, we summarize the main conclusions of our study.

2. THE PROJECTION SCHEME AND REDUCTION BY LEAST SQUARES

We start with the transport equation, for $0 < x < a$ and $-1 \leq \mu \leq 1$,

$$\mu\frac{\partial}{\partial x}\Psi(x,\mu) + \Psi(x,\mu) = \frac{c}{2}\sum_{l=0}^{L}\beta_l P_l(\mu)\int_{-1}^{1}P_l(\mu')\Psi(x,\mu')\mathrm{d}\mu' \tag{1}$$

and the boundary conditions, for $\mu > 0$,

$$\Psi(0,\mu) = F(\mu) \tag{2a}$$

and

$$\Psi(a,-\mu) = G(\mu), \tag{2b}$$

where $F(\mu)$ and $G(\mu)$ are considered known. As usual, c denotes the mean number of secondary particles emitted per collision and β_l, with $\beta_0 = 1$ and $|\beta_l| < 2l+1$, $l = 1, 2, \ldots, L$, are the coefficients in a Legendre expansion of the scattering law. In this paper we restrict our discussion to the case $c \leq 1$, i.e. that of a non-multiplying medium.

The essential idea behind the P_N method is that the first $N+1$ moments of Eq. (1) are satisfied by the P_N approximation, with N odd,

$$\Psi(x,\mu) = \sum_{n=0}^{N}\left(\frac{2n+1}{2}\right)\psi_n(x)P_n(\mu), \tag{3}$$

where $\psi_n(x)$, the n-th Legendre moment of the particle distribution function at position x, can be expressed, for $c < 1$, as (Benassi *et al.*, 1984)

$$\psi_n(x) = \sum_{j=1}^{J}\left[A_j e^{-x/\xi_j} + (-1)^n B_j e^{-(a-x)/\xi_j}\right]g_n(\xi_j). \tag{4}$$

Here $J = (N+1)/2$, $g_n(\xi)$ is the Chandrasekhar polynomial of order n, the eigenvalue ξ_j is the j-th positive zero of $g_{N+1}(\xi)$ and $\{A_j\}$ and $\{B_j\}$ are coefficients to be determined from the boundary conditions of the problem.

In the conservative case ($c = 1$), we note that one of the eigenvalues becomes infinite, and so the expression for the moments given by Eq. (4) must be modified (Benassi *et al.*, 1984). In what follows we consider $c < 1$; the required modifications for the case $c = 1$ are given in the Appendix of this paper.

We begin our development by noting that Eqs. (2) and (3) imply that, for $\mu > 0$,

$$\sum_{n=0}^{N} \left(\frac{2n+1}{2}\right) \psi_n(0) P_n(\mu) - F(\mu) = 0 \tag{5a}$$

and

$$\sum_{n=0}^{N} (-1)^n \left(\frac{2n+1}{2}\right) \psi_n(a) P_n(\mu) - G(\mu) = 0. \tag{5b}$$

Next we introduce the assumption that both $F(\mu)$ and $G(\mu)$ can be expressed by polynomial expansions of order $\leq N$. In the event that any of the incident particle distributions happens to have delta-function contributions, we can overcome this difficulty by decomposing the original problem into two problems: one for the uncollided and the other for the collided particle distribution function (Chandrasekhar, 1950). The uncollided problem can then be solved analytically and the collided problem does not involve delta-function incident distributions. With the above assumption about $F(\mu)$ and $G(\mu)$, the left-hand sides of Eqs. (5a) and (5b) are clearly polynomials of order N and, by projecting these equations against the shifted Legendre basis $\{P_k(2\mu - 1)\}$ and using Eq. (4) with $x = 0$ and $x = a$, we obtain, for $k = 0, 1, \ldots, N$,

$$\sum_{n=k}^{N} \left(\frac{2n+1}{2}\right) C_{k,n} \sum_{j=1}^{J} [A_j + (-1)^n B_j e^{-a/\xi_j}] g_n(\xi_j) = F_k \tag{6a}$$

and

$$\sum_{n=k}^{N} \left(\frac{2n+1}{2}\right) C_{k,n} \sum_{j=1}^{J} [(-1)^n A_j e^{-a/\xi_j} + B_j] g_n(\xi_j) = G_k, \tag{6b}$$

where we have defined

$$C_{k,n} = \int_0^1 P_k(2\mu - 1) P_n(\mu) \mathrm{d}\mu, \tag{7}$$

$$F_k = \int_0^1 P_k(2\mu - 1) F(\mu) \mathrm{d}\mu \tag{8a}$$

and

$$G_k = \int_0^1 P_k(2\mu - 1) G(\mu) \mathrm{d}\mu. \tag{8b}$$

Equations (6a) and (6b) constitute an overdetermined system of $2(N+1)$ algebraic equations for the $N+1$ unknown coefficients $\{A_j\}$ and $\{B_j\}$. It should be emphasized here that the fact that we are using a projection scheme based on an orthogonal basis on $[0, 1]$ is what causes the system of Eqs. (6a) and (6b) to be finite. A similar approach using the Marshak projection scheme would produce an infinite system that could be made finite only by truncation. Here we still have the problem that there are twice as many equations as there are unknowns, but, by using least squares to reduce the number of equations, we can keep, in an average sense, all the information given by Eqs. (6a) and (6b) for $k = 0, 1, \ldots, N$.

In order to show how to apply the least-squares technique to our overdetermined system, we prefer to use matrix notation. We thus write Eqs. (6a) and (6b) as

$$\mathbf{Ma} + \mathbf{NEb} = \mathbf{f} \tag{9a}$$

and

$$\mathbf{NEa} + \mathbf{Mb} = \mathbf{g}, \tag{9b}$$

where **M** and **N** are $(N+1)\times J$ matrices with elements given, for $i=1,2,\dots,N+1$ and $j=1,2,\dots,J$, respectively by

$$M_{i,j}=\sum_{n=i-1}^{N}\left(\frac{2n+1}{2}\right)C_{i-1,n}g_n(\xi_j) \tag{10a}$$

and

$$N_{i,j}=\sum_{n=i-1}^{N}(-1)^n\left(\frac{2n+1}{2}\right)C_{i-1,n}g_n(\xi_j), \tag{10b}$$

E is a $J\times J$ diagonal matrix with $\exp(-a/\xi_j)$, $j=1,2,\dots,J$, as elements, **a** and **b** are column vectors of dimension J with the unknown coefficients A_j and B_j, $j=1,2,\dots,J$, respectively as elements, and **f** and **g** are column vectors of dimension $N+1$ with elements $f_i=F_{i-1}$ and $g_i=G_{i-1}$, $i=1,2,\dots,N+1$, respectively. The system of equations expressed by Eqs. (9a) and (9b) can be written in a more compact form as

$$\mathbf{Px}=\mathbf{r}, \tag{11}$$

where

$$\mathbf{P}=\begin{pmatrix}\mathbf{M} & \mathbf{NE}\\ \mathbf{NE} & \mathbf{M}\end{pmatrix}, \tag{12}$$

$$\mathbf{x}=\begin{pmatrix}\mathbf{a}\\ \mathbf{b}\end{pmatrix} \tag{13}$$

and

$$\mathbf{r}=\begin{pmatrix}\mathbf{f}\\ \mathbf{g}\end{pmatrix}. \tag{14}$$

Our solution to the overdetermined system given by Eq. (11) is computed by the least-squares technique with equal weights (Jennings, 1977). The application of this technique reduces our problem to that of finding the solution of the *normal* equations, expressed by the square system of order $N+1$

$$\mathbf{P}^T\mathbf{Px}=\mathbf{P}^T\mathbf{r}. \tag{15}$$

Once this is done, the coefficients $\{A_j\}$ and $\{B_j\}$ become available and the particle distribution function could, in principle, be computed with Eqs. (3) and (4). However, it is well known (Garcia *et al.*, 1994a) that much improved results can be obtained by postprocessing Eq. (3) with the source-function integration technique (Kourganoff, 1952). The resulting postprocessed expression for the particle distribution function is given, for $\mu>0$, by

$$\Psi(x,\mu)=F(\mu)e^{-x/\mu}+\frac{c}{2}\sum_{l=0}^{K}\beta_lP_l(\mu)\Gamma_l(x,\mu) \tag{16a}$$

and

$$\Psi(x,-\mu)=G(\mu)e^{-(a-x)/\mu}+\frac{c}{2}\sum_{l=0}^{K}\beta_lP_l(\mu)\Gamma_l(x,-\mu), \tag{16b}$$

where $K=\min\{L,N\}$, and by defining

$$C(x:\mu,\xi)=\frac{e^{-x/\mu}-e^{-x/\xi}}{\mu-\xi} \tag{17a}$$

and

$$S(x:\mu,\xi)=\frac{1-e^{-x/\mu}e^{-x/\xi}}{\mu+\xi}, \tag{17b}$$

we can write $\Gamma_l(x, \pm\mu)$ as

$$\Gamma_l(x,\mu) = \sum_{j=1}^{J} \xi_j \left[A_j C(x:\mu,\xi_j) + (-1)^l B_j S(x:\mu,\xi_j) e^{-(a-x)/\xi_j}\right] g_l(\xi_j) \tag{18a}$$

and

$$\Gamma_l(x,-\mu) = \sum_{j=1}^{J} \xi_j \left[(-1)^l A_j S(a-x:\mu,\xi_j) e^{-x/\xi_j} + B_j C(a-x:\mu,\xi_j)\right] g_l(\xi_j). \tag{18b}$$

In addition to the particle distribution function, integrated quantities such as the total flux (we use here the terminology and notation of neutron transport theory)

$$\phi(x) = \int_{-1}^{1} \Psi(x,\mu)\mathrm{d}\mu, \tag{19}$$

the total current

$$J(x) = \int_{-1}^{1} \mu\Psi(x,\mu)\mathrm{d}\mu, \tag{20}$$

and the partial currents

$$J^{\pm}(x) = \int_{0}^{1} \mu\Psi(x,\pm\mu)\mathrm{d}\mu \tag{21}$$

may also be of interest when solving transport problems. In the P_N approximation, these quantities can be written in terms of the Legendre moments of the particle distribution function as

$$\phi(x) = \psi_0(x), \tag{22}$$

$$J(x) = \psi_1(x) \tag{23}$$

and

$$J^{\pm}(x) = \frac{1}{4}\psi_0(x) \pm \frac{1}{2}\psi_1(x) - \frac{1}{2}\sum_{m=1}^{J-1}(-1)^m(4m+1)\frac{(2m-3)!!}{(2m+2)!!}\psi_{2m}(x), \tag{24}$$

where the definition $(-1)!! = 1$ is to be used.

3. COMPUTATIONAL IMPLEMENTATION

In this section, we discuss several aspects relevant to the computational implementation of our shifted Legendre projection scheme.

We begin with the constants $C_{k,n}$ defined by Eq. (7). These constants can be computed in a fast and accurate way by using a recurrence relation derived, as shown below, with the help of some recurrence relations obeyed by the Legendre polynomials. We first let $n \Leftarrow n+1$ in Eq. (7) and multiply the resulting equation by $(n+1)$. We then let $n \Leftarrow n-1$ in Eq. (7), add the resulting equation multiplied by n to the previous result and use

$$(2n+1)P_n(\mu) = \left[\frac{\mathrm{d}}{\mathrm{d}\mu}P_{n+1}(\mu) - \frac{\mathrm{d}}{\mathrm{d}\mu}P_{n-1}(\mu)\right] \tag{25}$$

to obtain

$$(n+1)C_{k,n+1} + nC_{k,n-1} = \int_0^1 \mu P_k(2\mu-1)\left[\frac{\mathrm{d}}{\mathrm{d}\mu}P_{n+1}(\mu) - \frac{\mathrm{d}}{\mathrm{d}\mu}P_{n-1}(\mu)\right]\mathrm{d}\mu. \tag{26}$$

After an integration by parts, Eq. (26) yields

$$(n+2)C_{k,n+1}+(n-1)C_{k,n-1}=-\int_0^1 \mu\frac{\mathrm{d}}{\mathrm{d}\mu}P_k(2\mu-1)\,[P_{n+1}(\mu)-P_{n-1}(\mu)]\,\mathrm{d}\mu. \tag{27}$$

Letting $k \Leftarrow k+1$ in Eq. (27), subtracting the resulting equation from Eq. (27) and using

$$\mu\left[\frac{\mathrm{d}}{\mathrm{d}\mu}P_{k+1}(2\mu-1)-\frac{\mathrm{d}}{\mathrm{d}\mu}P_k(2\mu-1)\right]=(k+1)\,[P_{k+1}(2\mu-1)+P_k(2\mu-1)], \tag{28}$$

we obtain our final result, *viz.*

$$(n+k+3)C_{k+1,n+1}+(n-k-2)C_{k+1,n-1}=(n-k+1)C_{k,n+1}+(n+k)C_{k,n-1}. \tag{29}$$

Having in mind that $C_{k,n}=0$ for $k>n$, we can generate the required $C_{k,n}$, provided the first row is known, by using Eq. (29) row by row and adopting the convention that whenever a negative index occurs during the calculation, the corresponding element should be set equal to zero. With the help of Eq. (25), we can show by direct integration that the first row is given by

$$C_{0,n}=\left(\frac{1}{2n+1}\right)[P_{n-1}(0)-P_{n+1}(0)] \tag{30}$$

or, in a more explicit way, by $C_{0,0}=1$, $C_{0,1}=1/2$,

$$C_{0,2m}=0 \tag{31a}$$

and

$$C_{0,2m+1}=-\left(\frac{2m-1}{2m+2}\right)C_{0,2m-1}, \tag{31b}$$

for $m=1,2,\ldots$. Once the first row is computed, Eq. (29) can be used sequentially, as explained, to generate the remaining rows.

Additional computational aspects that should be mentioned here include the calculation of the P_N eigenvalues ξ_j, $j=1,2,\ldots,J$, and the corresponding Chandrasekhar polynomials $g_n(\xi_j)$, $n=0,1,\ldots,N$. In regard to the calculation of the P_N eigenvalues, we follow a procedure established in a previous work (Benassi *et al.*, 1984) that reduces this task to the calculation of the eigenvalues of a tridiagonal matrix of order J. The accurate calculation of the Chandrasekhar polynomials in high order has been the subject of a specific work (Garcia and Siewert, 1990).

Finally, in regard to the computational solution of the linear system given by Eq. (15), we recall that, since the matrix of coefficients $\mathbf{P}^T\mathbf{P}$ is positive definite, we are allowed to use particularly economical solution methods. For this purpose, we have elected to use subroutines DPOCO (or DPOFA) and DPOSL of the LINPACK package (Dongarra *et al.*, 1979).

4. NUMERICAL TESTS

In order to evaluate the performance of the proposed P_N boundary conditions, we have solved several basic half-space and slab problems and compared the numerical results of the shifted Legendre (SL) scheme to those of the Mark and Marshak schemes. We have verified that all three projection schemes are numerically stable in high order and that no scheme is better than the others for all problems. For each problem, the scheme with the best performance was found to depend on the input data (the parameter c, the scattering law order and coefficients, the incident particle distribution functions $F(\mu)$ and $G(\mu)$ and the slab thickness a) and also on the order of the approximation (N) used.

As an example of the kind of results we got, we show in Tables 1 to 4 the deviations of various orders of P_N approximations (using Marshak, Mark and SL boundary conditions) from the exact results found with the F_N method (Garcia *et al.*, 1994b) for the exit partial currents and total fluxes at the boundaries of a homogeneous layer defined by $c = 0.95$, $a = 1$, $L = 299$ and Mie scattering law coefficients that are given in Table 3 of Benassi *et al.* (1984). The boundary $x = 0$ of the layer is illuminated by an isotropic incident photon distribution specified by $F(\mu) = 1$, while the boundary $x = a$ is a free boundary, i.e. $G(\mu) = 0$.

Table 1. Percent Deviations of P_N Results for the Partial Current $J^-(0)$ in the Photon Transport Problem

N	Marshak	Mark	SL
3	-7.82	-11.7	-12.4
5	-2.52	-2.66	-0.99
7	-1.07	-0.76	0.50
9	-0.63	-0.30	0.44
19	-0.18	-0.066	-0.043
29	-0.074	-0.020	-0.032
39	-0.039	-0.0074	-0.017
99	-0.0052	0.0004	-0.0013
199	-0.0011	0.0004	0.0
299	-0.0005	0.0002	0.0002

Exact result: $J^-(0) = 0.0554611$

Table 2. Percent Deviations of P_N Results for the Total Flux $\phi(0)$ in the Photon Transport Problem

N	Marshak	Mark	SL
3	-5.06	-3.09	-1.43
5	-2.79	-1.28	0.31
7	-1.73	-0.61	0.69
9	-1.22	-0.35	0.68
19	-0.53	-0.12	0.31
29	-0.34	-0.075	0.19
39	-0.24	-0.051	0.14
99	-0.080	-0.011	0.060
199	-0.034	-0.0025	0.030
299	-0.021	-0.0008	0.020

Exact result: $\phi(0) = 1.19334$

Table 3. Percent Deviations of P_N Results for the Partial Current $J^+(a)$ in the Photon Transport Problem

N	Marshak	Mark	SL
3	0.95	1.81	1.90
5	0.28	0.48	0.26
7	0.12	0.18	0.034
9	0.070	0.097	0.021
19	0.023	0.024	0.032
29	0.0093	0.0090	0.017
39	0.0048	0.0045	0.0098
99	0.0005	0.0005	0.0015
199	0.0	0.0	0.0005
299	0.0	0.0	0.0003

Exact result: $J^+(a) = 0.398339$

Table 4. Percent Deviations of P_N Results for the Total Flux $\phi(a)$ in the Photon Transport Problem

N	Marshak	Mark	SL
3	8.78	7.11	5.43
5	4.05	2.77	0.90
7	2.15	1.18	-0.36
9	1.37	0.60	-0.61
19	0.60	0.18	-0.28
29	0.38	0.10	-0.18
39	0.27	0.067	-0.14
99	0.087	0.014	-0.062
199	0.037	0.0030	-0.031
299	0.023	0.0012	-0.021

Exact result: $\phi(a) = 0.689678$

By examining the results reported in Tables 1 to 4, we conclude that, for this problem, the convergence rate of the SL scheme is the best in low order, while in high order the convergence rate of the Mark scheme exceeds that of the other two schemes.

For the same problem, we show in Tables 5 and 6 our P_{299} results for the exit photon distribution function at $x = 0$ and at $x = a$ respectively, along with exact results generated with the F_N method that are thought to be accurate to within ± 1 in the last figure shown. As is usual with the P_N method, we observe that for all schemes the P_N results deviate from the exact results to a greater extent near $|\mu| = 0$; the largest deviations in the entries of Tables 5 and 6 for $\mu = 0$ are displayed by the Marshak scheme with

−0.29% and 0.61% respectively and the smallest by the Mark scheme with −0.023% and 0.052% respectively. The deviations of the SL scheme for $\mu = 0$ are comparable in magnitude to those of the Marshak scheme, although somewhat smaller (0.25% and −0.52%).

Table 5. Exact and P_{299} Results for $\Psi(0, -\mu)$ in the Photon Transport Problem

μ	Exact	Marshak	Mark	SL
0.0	0.678762	0.676795	0.678604	0.680431
0.01	0.611804	0.612264	0.612786	0.613162
0.05	0.513350	0.513374	0.513406	0.513426
0.1	0.445222	0.445228	0.445237	0.445244
0.2	0.333214	0.333216	0.333219	0.333222
0.3	0.243922	0.243924	0.243925	0.243926
0.4	0.178698	0.178698	0.178699	0.178699
0.5	0.132535	0.132535	0.132536	0.132536
0.6	0.100070	0.100071	0.100071	0.100071
0.7	0.0771522	0.0771522	0.0771523	0.0771525
0.8	0.0608134	0.0608135	0.0608135	0.0608136
0.9	0.0490996	0.0490997	0.0490997	0.0490996
1.0	0.0406760	0.0406760	0.0406760	0.0406758

Table 6. Exact and P_{299} Results for $\Psi(a, \mu)$ in the Photon Transport Problem

μ	Exact	Marshak	Mark	SL
0.0	0.199761	0.200989	0.199864	0.198727
0.01	0.242840	0.242555	0.242230	0.241997
0.05	0.312997	0.312982	0.312962	0.312951
0.1	0.371665	0.371662	0.371656	0.371654
0.2	0.490703	0.490702	0.490701	0.490702
0.3	0.601739	0.601738	0.601738	0.601740
0.4	0.689742	0.689742	0.689742	0.689744
0.5	0.755851	0.755851	0.755851	0.755853
0.6	0.804936	0.804936	0.804936	0.804937
0.7	0.841482	0.841482	0.841482	0.841483
0.8	0.868893	0.868893	0.868893	0.868894
0.9	0.889584	0.889584	0.889584	0.889584
1.0	0.905301	0.905301	0.905301	0.905301

5. CONCLUDING REMARKS

In this paper we have reported a shifted Legendre projection scheme for generating P_N boundary conditions free from ill-conditioning in high order, a deficiency found in an existing scheme (Garcia and Siewert, 1982) that is also based on the shifted Legendre polynomials.

In regard to the performance of the proposed scheme, we have concluded from our comparisons with the results of the Marshak and Mark projection schemes for several problems that none of the three schemes is more (or less) accurate than the others for all problems, a conclusion similar to that of a previous study that compared, in low order, variational and asymptotic P_N boundary conditions to Marshak and Mark boundary conditions (Rulko *et al.*, 1991).

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APPENDIX

Modifications for the Conservative Case

We report in this Appendix the modifications required in our formalism by the conservative case ($c = 1$). As mentioned in Sec. 2, one of the eigenvalues in Eq. (4) becomes infinite when $c = 1$, and so we follow Benassi *et al.* (1984) and replace Eq. (4) for $n = 0$ by

$$\psi_0(x) = A_1(a - x) + B_1 x + \sum_{j=2}^{J} \left[A_j e^{-x/\xi_j} + B_j e^{-(a-x)/\xi_j}\right], \tag{A.1a}$$

for $n = 1$ by

$$\psi_1(x) = (3 - \beta_1)^{-1}(A_1 - B_1), \tag{A.1b}$$

and for $n = 2, 3, \ldots, N$ by

$$\psi_n(x) = \sum_{j=2}^{J} \left[A_j e^{-x/\xi_j} + (-1)^n B_j e^{-(a-x)/\xi_j}\right] g_n(\xi_j), \tag{A.1c}$$

where ξ_j, $j = 2, 3, \ldots, J$, denote the *finite* eigenvalues.

If we now follow the procedure reported in Sec. 2 for the non-conservative case, we find that the linear system for the conservative case can still be expressed as in Eqs. (9a) and (9b), except that the first element of the diagonal matrix **E** is now given by 1, the elements of the first column of the **M** matrix by

$$M_{1,1} = \frac{a}{2} + \frac{3}{4}(3 - \beta_1)^{-1}, \tag{A.2a}$$

$$M_{2,1} = \frac{1}{4}(3 - \beta_1)^{-1} \tag{A.2b}$$

and, for $i = 3, 4, \ldots, N + 1$,

$$M_{i,1} = 0, \tag{A.2c}$$

and the elements of the first column of the **N** matrix by

$$N_{1,1} = -\frac{3}{4}(3 - \beta_1)^{-1}, \tag{A.3a}$$

$$N_{2,1} = -\frac{1}{4}(3 - \beta_1)^{-1} \tag{A.3b}$$

and, for $i = 3, 4, \ldots, N + 1$,

$$N_{i,1} = 0. \tag{A.3c}$$

In order to compute the P_N solutions, the expressions for the postprocessed particle distribution function given by Eqs. (16a) and (16b) can also be used for the conservative case, provided $\Gamma_l(x, \pm\mu)$ is defined, for $l = 0$, as

$$\Gamma_0(x,\mu) = A_1\left\{(a+\mu)\left[1 - e^{-x/\mu}\right] - x\right\} + B_1\left\{x - \mu\left[1 - e^{-x/\mu}\right]\right\} + \sum_{j=2}^{J} \xi_j\left[A_j C(x:\mu,\xi_j) + B_j S(x:\mu,\xi_j) e^{-(a-x)/\xi_j}\right] \tag{A.4a}$$

and

$$\Gamma_0(x,-\mu) = A_1\left\{a - x - \mu\left[1 - e^{-(a-x)/\mu}\right]\right\} + B_1\left\{x - a + (a+\mu)\left[1 - e^{-(a-x)/\mu}\right]\right\} + \sum_{j=2}^{J} \xi_j\left[A_j S(a-x:\mu,\xi_j) e^{-x/\xi_j} + B_j C(a-x:\mu,\xi_j)\right], \tag{A.4b}$$

for $l = 1$, as

$$\Gamma_1(x,\mu) = (A_1 - B_1)(3-\beta_1)^{-1}\left[1 - e^{-x/\mu}\right] \tag{A.5a}$$

and

$$\Gamma_1(x,-\mu) = (B_1 - A_1)(3-\beta_1)^{-1}\left[1 - e^{-(a-x)/\mu}\right], \tag{A.5b}$$

and, for $l = 2, 3, \dots, K$, as

$$\Gamma_l(x,\mu) = \sum_{j=2}^{J} \xi_j \left[A_j C(x:\mu,\xi_j) + (-1)^l B_j S(x:\mu,\xi_j) e^{-(a-x)/\xi_j}\right] g_l(\xi_j) \tag{A.6a}$$

and

$$\Gamma_l(x,-\mu) = \sum_{j=2}^{J} \xi_j \left[(-1)^l A_j S(a-x:\mu,\xi_j) e^{-x/\xi_j} + B_j C(a-x:\mu,\xi_j)\right] g_l(\xi_j). \tag{A.6b}$$

Finally, the integrated quantities defined in Sec. 2—total flux, total current and partial currents—can be expressed here as in Eqs. (22) to (24), but Eqs. (A.1a) to (A.1c) must be used to compute the required Legendre moments.