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Technical Note

A Note on the P_N Method with Mark Boundary Conditions

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Abstract — *The P_N solution for a half-space with isotropic scattering subject to an isotropic incident distribution is shown to yield, in any order, the exact scalar flux at the boundary when boundary conditions of the Mark type are used.*

I. INTRODUCTION

Recently,[1] during a study that compared different types of P_N boundary conditions for a few basic transport problems, we found numerical evidence that the P_N method with boundary conditions of the Mark type yields, in any order, the exact scalar flux at the boundary of an isotropically scattering half-space subject to an isotropic incident distribution. Because we are not aware of any previous mention of this result, we report here a proof that confirms our numerical observations.

II. THE PROOF

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

$$\mu \frac{\partial}{\partial x} \Psi(x,\mu) + \Psi(x,\mu) = \frac{c}{2} \int_{-1}^{1} \Psi(x,\mu') \, d\mu' \ , \quad (1)$$

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

$$\Psi(0,\mu) = 1 \quad (2a)$$

and

$$\lim_{x \to \infty} \Psi(x,-\mu) = 0 \ , \quad (2b)$$

where $\Psi(x,\mu)$ denotes the particle distribution function at position x and angle $\cos^{-1} \mu$ and where $c \in (0,1)$ denotes the mean number of secondary particles emitted per collision.

As is well known,[2] the first $N+1$ Legendre polynomial moments of Eq. (1) are satisfied by the P_N approximation (with N odd)

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

where, considering Eq. (2b), we have

$$\psi_n(x) = \sum_{j=1}^{J} A_j e^{-x/\xi_j} g_n(\xi_j) \ , \quad (4)$$

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

If we now use the Mark prescription for boundary conditions,[2,3] i.e., if we require that Eq. (2a) be satisfied at μ_i, $i = 1,2,\ldots,J$, the positive zeros of the Legendre polynomial $P_{N+1}(\mu)$, we obtain for $i = 1,2,\ldots,J$,

$$\sum_{j=1}^{J} A_j \sum_{n=0}^{N} \left(\frac{2n+1}{2}\right) P_n(\mu_i) g_n(\xi_j) = 1 \ , \tag{5}$$

a system of linear algebraic equations to be solved to determine the coefficients A_j, $j = 1,2,\ldots,J$. We now wish to show that we can derive an analytical expression for these coefficients. First, we specialize to isotropic scattering a more general relation reported by İnönü[4] to obtain

$$(\mu - \xi) \sum_{l=0}^{k} (2l+1) P_l(\mu) g_l(\xi) = (k+1)[P_{k+1}(\mu) g_k(\xi) - P_k(\mu) g_{k+1}(\xi)] - c\xi \ . \tag{6}$$

Using this result, we can rewrite Eq. (5) for $i = 1,2,\ldots,J$ as

$$\frac{c}{2} \sum_{j=1}^{J} A_j \left(\frac{\xi_j}{\xi_j - \mu_i}\right) = 1 \ . \tag{7}$$

We now define, in the manner of Chandrasekhar,[5]

$$H(-z) = \Gamma \frac{C(z)}{D(z)} \ , \tag{8}$$

where

$$C(z) = \prod_{k=1}^{J} (z - \mu_k) \ , \tag{9a}$$

$$D(z) = \prod_{k=1}^{J} (z - \xi_k) \ , \tag{9b}$$

and

$$\Gamma = \prod_{k=1}^{J} \left(\frac{\xi_k}{\mu_k}\right) \ . \tag{10}$$

In regard to $H(-z)$, we note that by using Cauchy's theorem, we can develop the alternative representation

$$H(-z) = \Gamma \left[1 + \sum_{k=1}^{J} \frac{C(\xi_k)}{(\xi_k - z) D'(\xi_k)}\right] \ . \tag{11}$$

In addition, considering that

$$P_{N+1}(z) = (-1)^J \frac{(2N+1)!!}{(N+1)!} C(z) C(-z) \tag{12a}$$

and for isotropic scattering

$$g_{N+1}(z) = (-1)^J (1-c) \frac{(2N+1)!!}{(N+1)!} D(z) D(-z) \ , \tag{12b}$$

we can show that the constant Γ can be written as

$$\Gamma = (1-c)^{-1/2} \ . \tag{13}$$

Proceeding with our proof, we use Eq. (11) for $z = \mu_i$, $i = 1,2,\ldots,J$, to obtain

$$\sum_{j=1}^{J} \frac{C(\xi_j)}{(\xi_j - \mu_i) D'(\xi_j)} = -1 \ . \tag{14}$$

By comparing this result to Eq. (7), we see that

$$A_j = -\left(\frac{2}{c}\right) \left[\frac{C(\xi_j)}{\xi_j D'(\xi_j)}\right] \tag{15}$$

for $j = 1,2,\ldots,J$, provided the linear system defined by Eq. (7) for $i = 1,2,\ldots,J$ has a unique solution. To prove that this is indeed the case, we start by using a sequence of elementary row and column matrix operations and algebraic manipulations of the type

$$\frac{\xi_k - \mu_j}{\xi_k - \mu_l} = 1 + \frac{\mu_l - \mu_j}{\xi_k - \mu_l} \tag{16}$$

to find that the determinant of the related matrix of coefficients,

$$\mathbf{M} = \frac{c}{2} \begin{bmatrix} \dfrac{\xi_1}{\xi_1 - \mu_1} & \dfrac{\xi_2}{\xi_2 - \mu_1} & \cdots & \dfrac{\xi_J}{\xi_J - \mu_1} \\ \dfrac{\xi_1}{\xi_1 - \mu_2} & \dfrac{\xi_2}{\xi_2 - \mu_2} & \cdots & \dfrac{\xi_J}{\xi_J - \mu_2} \\ \vdots & \vdots & \ddots & \vdots \\ \dfrac{\xi_1}{\xi_1 - \mu_J} & \dfrac{\xi_2}{\xi_2 - \mu_J} & \cdots & \dfrac{\xi_J}{\xi_J - \mu_J} \end{bmatrix} \ , \tag{17}$$

can be expressed as

$$|\mathbf{M}| = (-1)^{[J/2]} \left(\frac{c}{2}\right)^J \left(\prod_{1 \le i \le J} \xi_i\right) V(\mu_1, \mu_2, \mu_3, \ldots, \mu_J) \times V(\xi_1, \xi_2, \xi_3, \ldots, \xi_J) \left[\prod_{\substack{1 \le i \le J \\ 1 \le j \le J}} (\xi_i - \mu_j)\right]^{-1} \ , \tag{18}$$

where $[J/2]$ denotes the integer part of $J/2$ and

$$V(x_1, x_2, x_3, \ldots, x_J) = \begin{vmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^{J-1} \\ 1 & x_2 & x_2^2 & \cdots & x_2^{J-1} \\ 1 & x_3 & x_3^2 & \cdots & x_3^{J-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_J & x_J^2 & \cdots & x_J^{J-1} \end{vmatrix} \ . \tag{19}$$

Now, since the Vandermonde determinant given by Eq. (19) can be easily evaluated,[6] we can write Eq. (18) as

$$|\mathbf{M}| = (-1)^{[J/2]}\left(\frac{c}{2}\right)^J \left(\prod_{1\le i\le J} \xi_i\right)\left[\prod_{\substack{1<j\le J\\ 1\le k<j}} (\mu_j-\mu_k)\right] \times\left[\prod_{\substack{1<i\le J\\ 1\le l<i}} (\xi_i-\xi_l)\right]\left[\prod_{\substack{1\le i\le J\\ 1\le j\le J}} (\xi_i-\mu_j)\right]^{-1} . \quad (20)$$

Considering that the zeros of the Legendre polynomials are simple,[7] as are the zeros of the Chandrasekhar polynomials,[4] for $c \in (0,1)$, we can conclude from Eq. (20) that $|\mathbf{M}| \neq 0$ and thus the linear system defined by Eq. (7) for $i = 1,2,\ldots,J$ has, in fact, a unique solution.

Having found the required coefficients A_j, $j = 1,2,\ldots,J$, we can now compute the scalar flux at the boundary

$$\phi(0) = \int_{-1}^{1} \Psi(0,\mu)\, d\mu \ . \quad (21)$$

With the help of Eqs. (3), (4), and (15), we find

$$\phi(0) = -\left(\frac{2}{c}\right)\sum_{j=1}^{J} \frac{C(\xi_j)}{\xi_j D'(\xi_j)} \ . \quad (22)$$

This result can be simplified further if we set $z = 0$ in Eq. (11), use the resulting equation in Eq. (22), and note from Eqs. (8), (9), and (10) that $H(0) = 1$. We find

$$\phi(0) = \left(\frac{2}{c}\right)[1 - (1-c)^{1/2}] \ . \quad (23)$$

Finally, we can easily integrate Chandrasekhar's H-function solution to the half-space albedo problem[5] to verify that Eq. (23) is indeed the exact result for $\phi(0)$ in our problem.

III. CONCLUDING REMARKS

First, we note that by showing that the linear system defined by Eq. (7) has a unique solution, we have in fact shown that P_N solutions to isotropically scattering half-space problems are unique, regardless of the actual angular dependence of the incident distribution at $x = 0$, provided we use Mark's approach to generate the required conditions at the boundary. The case of a delta *function* incident distribution can be handled by decomposing the original problem into a problem for the uncollided flux that can be solved analytically and a problem for the collided flux that has a homogeneous boundary condition and an internal source.[5] As P_N particular solutions for problems with general internal sources are available in closed form,[8,9] it is clear that the P_N formulation for this second problem using Mark boundary conditions yields a linear system that has the same matrix of coefficients as Eq. (7).

We also note here that from a theoretical standpoint, it would be highly desirable to extend our uniqueness proof to other types of P_N boundary conditions, as for example, Marshak, and also to more difficult classes of problems, for example, finite media problems with anisotropic scattering.

Finally, we believe that the result proved in Sec. II for the scalar flux can be useful to users of the P_N method with boundary conditions of the Mark type as a simple check of the correctness of their numerical implementations, for isotropic scattering. We should also point out here that we have verified numerically that the special result that is the object of this technical note does not hold for other quantities of interest, as for example, the current and partial currents at the boundary. In addition, finding another transport problem where this (or a similar) result shows up does not seem to be an easy task.

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