JOURNAL OF COMPUTATIONAL PHYSICS 2, 197-205 (1967)

Difference Equations for the Legendre Polynomial Representation of the Transport Equation[1]

ROGER B. DEBAR

Lawrence Radiation Laboratory, University of California, Livermore, California 94550

ABSTRACT

The Legendre polynomial ("spherical harmonic") representation of the transport equation in plane and spherical symmetry is written in conservation form. Difference methods for the resultant equations are constructed and discussed.

I. INTRODUCTION

Solution of the time-dependent transport equation is of considerable interest in connection with problems in astrophysics and neutronics [1, 2]. Techniques for numerical integration of the equation have been a subject of investigation for the last two decades; this investigation was greatly aided by the development of large digital computers.

The intent of this paper is to investigate some of the properties of the Legendre polynomial ("spherical harmonic") representation of the one-dimensional transport equation with plane or spherical symmetry, and to difference the equations obtained.

II. THE LEGENDRE POLYNOMIAL REPRESENTATION

For simplicity we shall consider here only the special case of the frequency-independent radiative transport equation. The equation is:

$$\left[C^{-1}\frac{\delta}{\delta t} + \mu\frac{\delta}{\delta r} + \beta r^{-1}(1-\mu^2)\frac{\delta}{\delta \mu} + \sigma(r,t)\right] I(\mu,r,t) = S(\mu,r,t). \qquad (1)$$

Here $I(\mu, r, t)$ is the specific intensity at the angle $\cos^{-1}\mu$ at the spatial coordinate r and time t, C is the speed of light, $\sigma(r, t)$ is the total cross section, and $\beta = 0$

[1] Work performed under the auspices of the U.S. Atomic Energy Commission.

for plane symmetry while $\beta = 1$ for spherical symmetry. The source term $S(\mu, r, t)$ will not be explicitly specified; it is assumed to contain all effective sources including those due to scattering, etc. In the following discussion, derivatives with respect to r and t will often be denoted by subscripts.

Numerical integration techniques for Eq. (1) usually take the form of "Monte Carlo" calculations [3], discrete ordinate methods [4], or "moments" methods. The fundamentals of these approaches are fairly well known; they are discussed and compared by Campbell [5].

We shall deal here with the Legendre polynomial representation of Eq. (1), which belongs to the class of "moments" methods [6]. This representation can be obtained by multiplying Eq. (1) by $2\pi C^{-1}P_l(\mu)$, where $P_l(\mu)$ is the Legendre polynomial of order l, and integrating over the range $-1 \leqslant \mu \leqslant 1$, using the relations:

$$\begin{aligned} \mu P_l(\mu) &= \left(\frac{l+1}{2l+1}\right) P_{l+1}(\mu) + \left(\frac{l}{2l+1}\right) P_{l-1}(\mu) \\ (1-\mu^2)\, P_l'(\mu) &= -l[\mu P_l(\mu) - P_{l-1}(\mu)]. \end{aligned} \tag{2}$$

The result is an infinite set of coupled partial differential equations. In the usual spherical harmonics method, the sequence of equations is terminated by setting one of the Legendre polynomial integrals of $I(\mu, r, t)$ equal to zero. Here, however, we shall use a much more general terminal equation which arises from consideration of the transport equation in three dimensions [7]. This more general analysis leads uniquely to the choice of the Legendre polynomials as a basis for expansion of Eq. (1), and the truncated system of equations obtained has the very desirable property that the maximal velocity of signal propagation is exactly the same as that of Eq. (1); i.e., C.

If we define

$$\rho_l \equiv \rho_l(r, t) \equiv 2\pi C^{-1} \int_{-1}^{1} d\mu P_l(\mu)\, I(\mu, r, t), \tag{3}$$

$$S_l \equiv S_l(r, t) \equiv 2\pi C^{-1} \int_{-1}^{1} d\mu P_l(\mu)\, S(\mu, r, t), \tag{4}$$

then the system of equations, including the terminal relation, is

$$C^{-1}\rho_{0,t} + [\rho_{1,r} + 2\beta r^{-1}\rho_1] + \sigma\rho_0 = S_0\,, \tag{5}$$

$$\begin{aligned} C^{-1}\rho_{l,t} &+ \frac{l+1}{2l+1}[\rho_{l+1,r} + \beta(l+2)\, r^{-1}\rho_{l+1}] \\ &+ \frac{l}{2l+1}[\rho_{l-1,r} - \beta(l-1)\, r^{-1}\rho_{l-1}] + \sigma\rho_l = S_l\,; \quad l > 0, \end{aligned} \tag{6}$$

$$C^{-1}\rho_{2n-1,t} + [\rho_{2n-2,r} - 2\beta(n-1)\, r^{-1}\rho_{2n-2}] + \gamma_{2n-1}\sigma\rho_{2n-1} = \gamma_{2n-1}S_{2n-1}\,. \tag{7}$$

Here n may be any integer or half-integer greater than $\frac{1}{2}$, although for most practical purposes n is taken to be integral. In the time-independent limit of Eq. (7) when $n = 1$, γ_1 is the reciprocal of the diffusion constant. In general we have

$$\gamma_{2n-1} = \frac{4n - 1}{2n(1 + \alpha_{2n-2}) - 1}, \tag{8}$$

where $\alpha_{2n-2} \equiv \alpha_{2n-2}(r, t)$ is essentially the parameter introduced by Pomraning [8].

In cases where $\alpha_{2n-2}(r, t)$ is independent of $I(\mu, r, t)$, it can be evaluated by the formula

$$\alpha_{2n-2}(r, t) = \frac{\int_{-1}^{1} d\mu\, P_{2n}(\mu)\, \tilde{I}(\mu, r, t)}{\int_{-1}^{1} d\mu\, P_{2n-2}(\mu)\, \tilde{I}(\mu, r, t)}, \tag{9}$$

where $\tilde{I}(\mu, r, t)$ is an assumed approximation to the *plane-symmetric* intensity distribution.

For example, in the asymptotic limit we have

$$\tilde{I}(\mu, r, t) \to \frac{A_1(r, t)}{1 + K\mu} + \frac{A_2(r, t)}{1 - K\mu} \tag{10}$$

where $K \equiv K(r, t)$ is related to the constant $D(r, t)$ of asymptotic diffusion theory by: $D(r, t) = (1 - K/\tanh^{-1}K)/K^2$. Substitution of Eq. (10) into Eq. (9) gives

$$\alpha_{2n-2}(r, t) \to \frac{\int_0^1 d\mu\, P_{2n}(\mu)(1 - K^2\mu^2)^{-1}}{\int_0^1 d\mu\, P_{2n-2}(\mu)(1 - K^2\mu^2)^{-1}} \tag{11}$$

for the usual case where n is integral [8].

III. The Conservative Representation

There are clearly many ways of writing difference equations corresponding to Eqs. (5–7). We wish to write a difference scheme that will preserve the conservation properties of the differential equations. ("Conserved quantities" will be considered to be quantities which, except for explicit sources and sinks, are conserved when integrated over a bounded system.)

For plane symmetry all the ρ_l are conserved, but for spherical symmetry and n integral, there are exactly as many essentially uniquely determined conserved linear combinations of the ρ_l as there are equations. This is not true for n half-integral; in general, the existing conservation conditions do not saturate the equations, nor are they unique. We shall accordingly restrict our investigation to the case of integral n.

Let:

$$E(W_l) \equiv \sum_{l=0}^{2n-1} W_l \rho_l \tag{12}$$

First we choose $W_{2l-1} = 0$; $l = 1, 2,..., n$ and arbitrarily $W_0 = 1$. Then for each of the values of the parameter $m = 1, 2,..., n$ we apply the recursion relation:

$$W_{l+2}^m = W_l^m \left[\frac{(l+1)(2l+5)}{(l+2)(2l+1)} \left\{\frac{(l+2) - 2m}{(l+1) + 2m}\right\}\right], \tag{13}$$

to obtain a total of n conserved quantities:

$$r^{2\beta m} E(W_l^m). \tag{14}$$

Neglecting sources and sinks, the quantities $E(W_l^m)$ obey differential equations of the form:

$$\frac{\delta}{\delta t} E(W_l^m) + r^{-2\beta m} \frac{\delta}{\delta r} [r^{2\beta m} F^m] = 0, \tag{15}$$

where F^m is another linear combination of the ρ_l.

Next, we choose $W_{2l} = 0$; $l = 0, 1,..., n-1$ and arbitrarily $W_{2n-1} = 1$. Then for each of the values of the parameter $m = 0, -1, -2,..., -(n-1)$ we apply the relations:

$$W_{2n-3}^m = W_{2n-1}^m \left[\frac{4n-5}{n-1} \left\{\frac{(n-1) + m}{(2n-1) - 2m}\right\}\right], \tag{16}$$

$$W_{l-2}^m = W_l^m \left[\frac{l(2l-3)}{(l-1)(2l+1)} \left\{\frac{(l-1) + 2m}{l - 2m}\right\}\right]; \qquad l < 2n-1, \tag{17}$$

to obtain another n conserved quantities of the form (14) satisfying equations of the form (15).

This prescription can be easily derived by forming linear combinations of Eqs. (5–7). If the coefficients of the linear combinations of the $\rho_{l,t}$ are W_l, we will obtain expressions of the form:

$$C^{-1} \frac{\delta}{\delta t} E(W_l) + \sum_{l=0}^{2n-2} a_l [\rho_{l,r} + b_l \beta r^{-1} \rho_l] = \text{source and sink terms},$$

where a_l and b_l are functions of the W's. The W_l given in Eqs. (13), (16), and (17) are just those which make b_l independent of l. The algebraic details (which also lead automatically to the demonstration of uniqueness) are straightforward and will not be given here. Instead, we shall give an example of the method for the case $n = 2$.

Application of Eq. (13) yields

$$m = 1: \{W_0 \equiv 1; \quad \text{all other} \quad W_l = 0\},$$

$$m = 2: \{W_0 \equiv 1; W_2 = -1; \quad \text{all other} \quad W_l = 0\}.$$

Next, application of Eqs. (16) and (17) gives

$$m = 0: \{W_3 \equiv 1; W_1 = 1; \quad \text{all other} \quad W_l = 0\},$$

$$m = -1: \{W_3 \equiv 1; \quad \text{all other} \quad W_l = 0\}.$$

Then the appropriate conservative differential equations are:

$$C^{-1}\rho_{0,t} + r^{-2\beta} \frac{\delta}{\delta r} [r^{2\beta}\rho_1] + \sigma\rho_0 = S_0 , \tag{18}$$

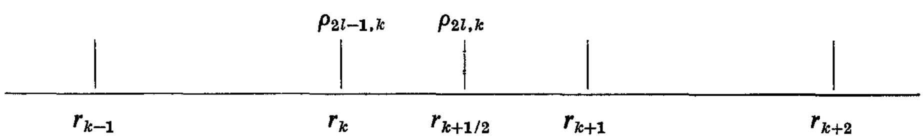
$$C^{-1}(\rho_0 - \rho_2)_t + \frac{3}{5} r^{-4\beta} \frac{\delta}{\delta r} [r^{4\beta}(\rho_1 - \rho_3)] + \sigma(\rho_0 - \rho_2) = S_0 - S_2 , \tag{19}$$

$$C^{-1}(\rho_1 + \rho_3)_t + \frac{1}{3} \frac{\delta}{\delta r} (\rho_0 + 5\rho_2) + \sigma(\rho_1 + \gamma_3\rho_3) = S_1 + \gamma_3 S_3 , \tag{20}$$

$$C^{-1}\rho_{3,t} + r^{2\beta} \frac{\delta}{\delta r} [r^{-2\beta}\rho_2] + \gamma_3\sigma\rho_3 = \gamma_3 S_3 . \tag{21}$$

IV. Space Difference Equations

Once our differential equations have been written in conservation form, we can difference them in such a way as to preserve their conservation properties. Let us consider a spatial mesh in which the ρ_{2l-1} ; $l = 1, 2, \ldots, n$ are "centered" at the zone boundaries r_k and the ρ_{2l} , $l = 0, 1, \ldots, n - 1$ are "centered" at the points $r_{k+1/2} \sim \frac{1}{2}(r_{k+1} + r_k)$.



Then if E is centered at $k + \frac{1}{2}$, F will be centered at k, and we can integrate Eq. (15) as follows:

$$\frac{\delta}{\delta t} \int_{r_k}^{r_{k+1}} dr\, r^{2\beta m} E(r) + r_{k+1}^{2\beta m} F_{k+1} - r_k^{2\beta m} F_k = 0.$$

Our difference equations will be reasonably well "centered" and the conservation laws will be satisfied if we take $E(r) \to E_{k+1/2}$; $r_k < r < r_{k+1}$. Then the difference equation is:

$$\frac{\delta}{\delta t} E_{k+1/2} + (2\beta m + 1)(r_{k+1}^{2\beta m+1} - r_k^{2\beta m+1})^{-1}(r_{k+1}^{2\beta m} F_{k+1} - r_k^{2\beta m} F_k) = 0. \tag{22}$$

If, on the other hand, E is centered at k and F at $k + \frac{1}{2}$, the appropriate difference equation can be obtained from Eq. (22) simply by substituting $k \to k - \frac{1}{2}$ everywhere.

For the system of Eqs. (18–21), we obtain:

$$\begin{aligned} C^{-1} \frac{\delta}{\delta t} \rho_{0,k+1/2} &+ (1 + 2\beta)(r_{k+1}^{1+2\beta} - r_k^{1+2\beta})^{-1}[r_{k+1}^{2\beta} \rho_{1,k+1} - r_k^{2\beta} \rho_{1,k}] \\ &+ \sigma_{k+1/2} \rho_{0,k+1/2} = S_{0,k+1/2} , \end{aligned} \tag{23}$$

$$\begin{aligned} C^{-1} \frac{\delta}{\delta t} (\rho_{0,k+1/2} - \rho_{2,k+1/2}) &+ \frac{3}{5}(1 + 4\beta)(r_{k+1}^{1+4\beta} - r_k^{1+4\beta})^{-1} \\ &\times [r_{k+1}^{4\beta}(\rho_{1,k+1} - \rho_{3,k+1}) - r_k^{4\beta}(\rho_{1,k} - \rho_{3,k})] \\ &+ \sigma_{k+1/2}(\rho_{0,k+1/2} - \rho_{2,k+1/2}) = S_{0,k+1/2} - S_{2,k+1/2} , \end{aligned} \tag{24}$$

$$\begin{aligned} C^{-1} \frac{\delta}{\delta t} (\rho_{1,k} + \rho_{3,k}) &+ \frac{1}{3}(r_{k+1/2} - r_{k-1/2})^{-1}[(\rho_{0,k+1/2} + 5\rho_{2,k+1/2}) \\ &- (\rho_{0,k-1/2} + 5\rho_{2,k-1/2})] + \sigma_k(\rho_{1,k} + \gamma_{3,k}\rho_{3,k}) = S_{1,k} + \gamma_{3,k} S_{3,k} , \end{aligned} \tag{25}$$

$$\begin{aligned} C^{-1} \frac{\delta}{\delta t} \rho_{3,k} &+ (1 - 2\beta)[r_{k+1/2}^{1-2\beta} - r_{k-1/2}^{1-2\beta}]^{-1}[r_{k+1/2}^{-2\beta} \rho_{2,k+1/2} - r_{k-1/2}^{-2\beta} \rho_{2,k-1/2}] \\ &+ \gamma_{3,k} \sigma_k \rho_{3,k} = \gamma_{3,k} S_{3,k} . \end{aligned} \tag{26}$$

(Precise definitions of σ_k , $\sigma_{k+1/2}$, $S_{l,k}$, $S_{l,k+1/2}$ and $\gamma_{3,k}$ are not needed for the purposes of this discussion.)

If, now, these equations are rearranged to yield difference expressions similar to our original Eqs. (5–7) for $n = 2$, the resultant formulas are considerably different in detail from any one would be inclined to write "naturally." One of the advantages of the conservation equation approach is that it greatly limits the variety of space differencing schemes one must consider.

It should also be mentioned that boundary conditions are especially easy to deal with in this representation. The most natural conditions are specification of all the ρ_l initially, together with the appropriate fluxes of the conserved quantities for later times at the boundaries $r_{k\min}$ and $r_{k\max}$. (This is similar to Marshak [9] boundary conditions in that the ρ_l of odd order are specified on the outer boundaries of the system. For example, Eqs. (23–26) would require specification of ρ_1 and $(\rho_1 - \rho_3)$ at $k = k\min$ and $k = k\max$.)

Other conservative differencing schemes are of course possible; for example, we could have chosen to center all the ρ_l at k. Then Eq. (22) would be replaced by:

$$\frac{\delta}{\delta t} E_k + \frac{1}{2}(2\beta m + 1)(r_{k+1}^{2\beta m+1} - r_{k-1}^{2\beta m+1})^{-1} \times [r_{k+1}^{2\beta m} F_{k+1} - r_{k-1}^{2\beta m} F_{k-1}] = 0.$$

This "leapfrog" differencing scheme, however, has a space differencing error equivalent to that of the "staggered" scheme given earlier, used with double the mesh spacing. It is therefore less accurate; in fact, for equivalent mesh spacings the formal error estimate is four times as great, since for plane symmetry the differencing error is of order $(\Delta r)^2$.

V. Time Differencing

The space-differenced equations for the ρ_l can be written in a very compact symbolic form if we define

$$\boldsymbol{\rho}_k \equiv \begin{pmatrix} \rho_{0,k+1/2} \\ \rho_{1,k} \\ \rho_{2,k+1/2} \\ \vdots \\ \rho_{2n-1,k} \end{pmatrix}, \qquad \boldsymbol{S}_k \equiv \begin{pmatrix} S_{0,k+1/2} \\ S_{1,k} \\ S_{2,k+1/2} \\ \vdots \\ S_{2n-1,k} \end{pmatrix}, \tag{27}$$

where now the $S_{2l,k+1/2}$ and $S_{2l-1,k}$ are taken to include only the "true" sources, and not the effective sources due to scattering. Then, where $M_{m,k}$; $m = -1, 0, 1$ are three $2n \times 2n$ matrices which contain all the coefficients of the ρ_l in the space-differenced equations, including those due to scattering extracted from the S_l, we have

$$C^{-1}\boldsymbol{\rho}_{k,t} + \sum_{m=-1}^{1} M_{m,k}\boldsymbol{\rho}_{k+m} = \boldsymbol{S}_k . \tag{28}$$

Next we write a time-differenced equation corresponding to Eq. (28):

$$(C\Delta t^{n+1/2})^{-1}(\boldsymbol{\rho}_k^{n+1} - \boldsymbol{\rho}_k^{n}) + \sum_{m=-1}^{1} M_{m,k}^{n+1/2}(\theta^1\boldsymbol{\rho}_{k+m}^{n+1} + \theta^0\boldsymbol{\rho}_{k+m}^{n}) = \boldsymbol{S}_k^{n+1/2}, \tag{29}$$

where

$$\rho_l^n \equiv \rho_l(t^n), \text{ etc.,} \quad \Delta t^{n+1/2} \equiv t^{n+1} - t^n,$$

and normally

$$0 \leqslant \theta^0 \leqslant 1; \qquad \theta^1 = 1 - \theta^0.$$

Quantities "centered" at $t^{n+1/2}$, such as $S_k^{n+1/2}$, are to be evaluated in some reasonable manner. They must, however, be treated as constants throughout the time interval $t^n \leqslant t \leqslant t^{n+1}$.

Equation (29) can now be solved by the tridiagonal algorithm [10, 11], except that here the coefficients appearing in the algorithm are $2n \times 2n$ matrices, and must be treated accordingly. For small values of n the matrices are not difficult to evaluate, especially since they tend to be sparse.

The obvious choices for θ^0 and θ^1 in Eq. (29) are

$$\{\theta^0 = 0;\ \theta^1 = 1\} \qquad \text{and} \qquad \{\theta^1 = \theta^0 = \tfrac{1}{2}\}.$$

Unfortunately, the first of these schemes introduces unphysical damping effects, as is often the case in "pure implicit" systems, while the second choice does not damp short wavelengths for large values of the diffusion parameter $[\sigma\Delta t/(\Delta r)^2]$. Again, this is common in the case of such "Crank-Nicholson" systems.

A scheme which is no more difficult in principle to use than is the "Crank-Nicholson" but which has much better damping properties may be characterized in the following manner. Various difference approximations to the differential equation $f_t + Hf = 0$, where H is a time-independent operator, may be obtained by making rational approximations to the exponential in the exact solution:

$$f^{n+1} = \exp(-x) f^n; \qquad \text{where} \qquad x \equiv H\Delta t^{n+1/2}.$$

For example, the approximation similar to that given in Eq. (29) would be

$$\exp(-x) \approx (1 + \theta^1 x)^{-1}(1 - \theta^0 x).$$

The operator we shall consider is of the form

$$\exp(-x) \approx [1 + (1 - \tfrac{1}{2}\sqrt{2})x]^{-1}[1 - (\sqrt{2} - 1)x][1 + (1 - \tfrac{1}{2}\sqrt{2})x]^{-1}. \quad (30)$$

It can be shown that this operator approximates $\exp(-x)$ correctly through terms of order x^2, as does the Crank-Nicholson operator. Furthermore, in the diffusion limit, where x yields a large positive eigenvalue, this approximation approaches zero from below and has good damping properties everywhere, whereas the Crank-Nicholson operator does not.

The calculational procedure, then, is to hold $M_{m,k}^{n+1/2}$ and $S_k^{n+1/2}$ fixed while solving Eq. (29) with

$$\{\Delta t^{n+1/2} \to (1 - \tfrac{1}{2}\sqrt{2})\,\Delta t^{n+1/2};\ \theta^0 \to 0;\ \theta^1 \to 1\}.$$

Next, still holding $M_{m,k}^{n+1/2}$ and $S_k^{n+1/2}$ at the same values, and operating upon the result of the calculation just completed, solve Eq. (29) again with:

$$\{\Delta t^{n+1/2} \to \tfrac{1}{2}\sqrt{2}\,\Delta t^{n+1/2};\ \theta^0 \to 2 - \sqrt{2};\ \theta^1 \to \sqrt{2} - 1\}.$$

Experimentally, this technique has behaved as expected; it appears to have none of the damping error behavior associated with the Crank-Nicholson operator. The latter operator should be quite acceptable for many purposes, however, and is somewhat less complicated and time-consuming than that given in Eq. (30).

In the case of plane symmetry and constant coefficients, it is possible to demonstrate that this method is unconditionally stable, and no instabilities have been observed in experiments with systems of equations of order $2n = 4$. Further numerical experiments are in progress to investigate the accuracy of this technique in comparison with other methods of equivalent computational complexity. It is suggested that the extent to which the conservation rules derived above are satisfied by other difference methods for the Legendre polynomial Eqs. (5–7) could constitute a check on the overall accuracy of such schemes; such checks are also quite useful in program debugging.

REFERENCES

1. R. D. Richtmyer, "Difference Methods for Initial Value Problems," pp. 121–125. Wiley (Interscience), New York (1957).
2. S. Chandrasekhar, "An Introduction to the Study of Stellar Structure." Dover, New York (1957).
3. J. A. Fleck, *in* "Methods in Computational Physics," Vol. I, pp. 43–65. Academic Press, New York (1963).
4. R. D. Richtmyer, (Ref. [1], pp. 137–139; 141–151).
5. P. M. Campbell, "Finite Difference Methods for Nonlinear Radiation Transport," Univ. of California Radiation Laboratory, UCRL–12411.
6. R. D. Richtmyer, (Ref. [1], pp. 127–137; 139–141).
7. R. B. DeBar, "Truncation of the Spherical Harmonic Expansion of the Transport Equation," *Nucl. Sci. Eng.* **30**, 159–165 (1967).
8. G. C. Pomraning, *Nukleonik 6*, 348 (1965).
9. R. Marshak, *Phys. Rev.* **71**, 443 (1947).
10. R. D. Richtmyer, (Ref. [1] pp. 101–104).
11. B. Wendroff, "Theoretical Numerical Analysis," pp. 28–29. Academic Press, New York (1966).

Printed in Belgium