M&C 2001 Salt Lake City, Utah, USA, September 2001.

INFINITE MEDIUM SOLUTIONS OF THE TRANSPORT EQUATION, S_N DISCRETIZATION SCHEMES, AND THE DIFFUSION APPROXIMATION

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Keywords: neutron transport, discrete ordinates, spatial discretization schemes, diffusion approximation

ABSTRACT

A family of solutions of the infinite-medium transport equation is constructed. This family consists of angular fluxes, which are linear (or quadratic) in space and angle, and which are driven by isotropic sources that are linear (or quadratic) in space. We show that each angular flux in this family satisfies Fick's Law; thus, the corresponding scalar flux satisfies the standard diffusion equation. We also show that (*i*) only certain transport discretization schemes preserve the "linear" infinite-medium solutions, and (*ii*) these schemes are more accurate in diffusive problems. We specifically show that the discrete "quadratic" solutions of these schemes are much more accurate for problems in which the cell width is not optically thin. The contents of this paper demonstrate why it is advantageous for spatial differencing schemes to preserve the "linear" (as well as the "flat") infinite-medium solutions of the transport equation.

1. INTRODUCTION

In developing discretization methods for the transport equation, several considerations enable one to assess the accuracy and robustness of a proposed scheme (Alcouffe, 1979), (Lewis, 1984). Does the scheme satisfy particle balance? Does it preserve the "infinite-medium" (flat isotropic source, flat isotropic angular flux) solution? In 1-D, is the scheme at least second-order accurate? If the source is positive, is the resulting angular flux necessarily positive? Does the scheme satisfy the "diffusion limit" (Larsen, 1987), (Larsen, 1992)? This last question is one of the most theoretically difficult, particularly for multidimensional problems with an unstructured spatial grid (Adams, 1998), (Adams, 2001), (Wareing, 1999). In this paper, an expanded version of a recent ANS abstract (Larsen, 2001), we develop a new theoretical technique to address this question.

The new technique makes use of a certain family of infinite-medium solutions of the transport equation. This family consists of angular fluxes, which are linear (or quadratic) in space and angle, and which are driven by sources that are linear (or quadratic) in space. Because of the structure of these angular fluxes, they satisfy Fick's Law, even though they are not always linear in angle. Thus, for each angular flux in this family, the corresponding scalar flux satisfies the standard diffusion equation. (In a finite medium, the standard diffusion equation would predict the exact scalar flux if "exact" diffusion boundary conditions were employed.)

Now, we ask: how well does a given transport discretization scheme reproduce these exact solutions? All reasonable discretization schemes preserve the “flat” (flat isotropic source, flat isotropic flux) solution for all space-angle grids. Also, all reasonable discretization schemes reproduce any exact solution in the fine-mesh limit. However, not all discretization schemes preserve even the “linear” solution on all grids. What are the consequences of a discretization scheme preserving (or not preserving) the “linear” solution for all grids?

The purpose of this paper is to explore and partly answer this question. In planar geometry, we show that among the class of weighted-diamond discretizations of the standard S_N equations, only the conventional Diamond Difference scheme preserves the linear solution for all space-angle grids. The weighted-diamond “linear” solutions have a truncation error in the cell-edge angular flux. This produces a truncation error in Fick’s Law, which in turn produces a truncation error in the discrete “quadratic” solution. Diamond solutions do not possess this particular error. Thus, the inability of the weighted-diamond schemes to preserve the “linear” solution is directly linked to a significant loss of accuracy in diffusive problems.

This demonstrates that it is advantageous for a transport differencing scheme to preserve the exact “linear” transport solutions for all space-angle grids: possession of this property enables an accurate discrete form of Fick’s law to hold in problems for which the angular flux is nearly linear in angle. A second likely benefit is that the numerical solution will be overall more grid-independent. These two properties enable the computational solution to be more accurate in diffusive problems with weak spatial and angular dependence.

The work in this paper directly relates to “characteristic” methods that are presently employed in S_N reactor lattice physics codes (Knott, 1995), (Hong, 1998). A typical such method is the “Step Characteristic” scheme, in which the scattering source is approximated as a spatial histogram and the S_N equations are solved analytically along characteristic lines passing through the system in discrete-ordinates directions (Alcouffe, 1979). This method has several attractive features: the solution is positive and the representation of the scattering source requires minimal storage; in planar geometry the solution is second-order accurate, and is exact in a pure absorber with a histogram interior source. The Diamond-Difference solution requires the same storage and in 1-D is second-order accurate, but is not always positive and is not exact in a pure absorber. Also, the Diamond solution can exhibit unphysical spatial oscillations in absorbing regions unless the spatial grid is optically thin, whereas the Step Characteristic scheme behaves “monotonically.”

Nonetheless, the analysis in this paper shows that the Diamond Difference solution is more accurate for “diffusive” neutron transport problems. The root cause of this is that the Step Characteristic scheme fails to preserve the “linear” transport solution. As described below, this leads to an unphysically large “effective diffusion coefficient” for spatial grids that are not optically thin.

The remainder of this paper is organized as follows. In Section 2 we construct “linear” and “quadratic” infinite-medium solutions for 1-D planar and spherical geometries. In Section 3 we consider weighted diamond planar-geometry S_N differencing schemes and show that only the conventional Diamond Difference scheme preserves the “linear” solution for all space-angle grids. We also show that schemes that preserve the linear solution produce significantly more accurate “quadratic” solutions on space-angle grids that are not optically thin. In Section 4 we discuss related issues in spherical geometry. We conclude in Section 5 with a discussion.

2. INFINITE-MEDIUM TRANSPORT SOLUTIONS

Our analysis applies to the mono-energetic 3-D transport equation:

$$\underline{\Omega}\cdot\underline{\nabla}\Psi(\underline{r},\underline{\Omega})+\Sigma_t\Psi(\underline{r},\underline{\Omega}) = \int_{4\pi}\Sigma_s(\underline{\Omega}\cdot\underline{\Omega}')\Psi(\underline{r},\underline{\Omega}')d\Omega' + \frac{1}{4\pi}Q(\underline{r}) \ , \tag{1}$$

where

$$\underline{r} = (x,y,z) = \text{spatial variable} \ , \tag{2}$$

$$\underline{\Omega} = (\mu,\eta,\xi) = \text{angular variable} \ , \tag{3}$$

and

$$\Sigma_s(\mu_0) = \sum_{k=0}^{\infty}\frac{2k+1}{4\pi}\Sigma_{sk}P_k(\mu_0) = \text{differential scattering cross section} \ , \tag{4}$$

with $\mu_0 = \underline{\Omega}\cdot\underline{\Omega}'$ and P_k = the k^{th} Legendre polynomial.

2.1 Planar Geometry

We first consider a planar-geometry problem with spatial variation only in the x-direction:

$$Q(\underline{r}) = q(x) \ , \tag{5}$$

$$\Psi(\underline{r},\underline{\Omega}) = \frac{1}{2\pi}\psi(x,\mu) \ . \tag{6}$$

Eq. (1) simplifies to

$$\mu\frac{\partial\psi}{\partial x}(x,\mu)+\Sigma_t\psi(x,\mu) = \int_{-1}^{1}\Sigma_s(\mu,\mu')\psi(x,\mu')d\mu' + \frac{q(x)}{2} \ , \tag{7}$$

with

$$\Sigma_s(\mu,\mu') = \sum_{k=0}^{\infty}\frac{2k+1}{2}\Sigma_{sk}P_k(\mu)P_k(\mu') \ . \tag{8}$$

We now construct a family of “infinite-medium” solutions of Eq. (7), in which the prescribed source and angular flux are spatially quadratic:

$$q(x) = q_0+q_1x+q_2x^2 \ , \tag{9}$$

$$\psi(x,\mu) = \psi_0(\mu)+\psi_1(\mu)x+\psi_2(\mu)x^2 \ , \tag{10}$$

with functions $\psi_j(\mu)$ to be determined. Introducing Eqs. (9) and (10) into Eq. (7) and equating the coefficients of x^j, we obtain for $j = 0,1,$ and 2

$$\Sigma_t\psi_j(\mu) - \int_{-1}^{1}\Sigma_s(\mu,\mu')\psi_j(\mu')d\mu' = \frac{q_j}{2} - (j+1)\mu\psi_{j+1}(\mu) \ , \tag{11}$$

with $\psi_3(\mu) = 0$. These equations can be solved recursively, first for $j = 2$, then for $j = 1$, and then $j = 0$.

The $j = 2$ solution is isotropic:

$$\psi_2(\mu) = \frac{q_2}{\Sigma_{a0}} \ . \tag{12}$$

(We employ the notation

$$\Sigma_{an} \equiv \Sigma_t - \Sigma_{sn} \ , \ n = 0, 1, 2 \ , \tag{13}$$

which implies that $\Sigma_{a0} = \Sigma_a$ = absorption cross section and $\Sigma_{a1} = \Sigma_{tr}$ = transport cross section. For now, we assume $\Sigma_{a0} \neq 0$.) The $j = 1$ solution is linear in μ:

$$\psi_1(\mu) = \frac{1}{2\Sigma_{a0}} \left(q_1 - 2\mu \frac{q_2}{\Sigma_{a1}} \right) \ , \tag{14}$$

and the $j = 0$ solution is quadratic in μ:

$$\psi_0(\mu) = \frac{1}{\Sigma_{a0}} \left(\frac{q_0}{2} + \frac{q_2}{3\Sigma_{a1}\Sigma_{a0}} \right) - \left(\frac{q_1}{2\Sigma_{a1}\Sigma_{a0}} \right) \mu + \left(\frac{2q_2}{3\Sigma_{a1}\Sigma_{a2}\Sigma_{a0}} \right) P_2(\mu) \ . \tag{15}$$

Introducing Eqs. (12), (14), and (15) into (10), we obtain:

$$\begin{aligned} \psi(x,\mu) \ &= \ \frac{q_0}{2\Sigma_{a0}} + \left(x - \frac{\mu}{\Sigma_{a1}} \right) \frac{q_1}{2\Sigma_{a0}} \\ &+ \ \left[x^2 - \frac{2\mu x}{\Sigma_{a1}} + \frac{2}{3\Sigma_{a1}} \left(\frac{1}{\Sigma_{a0}} + \frac{3\mu^2 - 1}{\Sigma_{a2}} \right) \right] \frac{q_2}{2\Sigma_{a0}} \ , \end{aligned} \tag{16}$$

which is a second-order polynomial in x and μ. This angular flux, which is driven by the source $q(x)$ in Eq. (9), has the following scalar flux and current:

$$\phi(x) \equiv \int_{-1}^{1} \psi(x,\mu) d\mu = \frac{1}{\Sigma_{a0}} \left[q(x) + \frac{2q_2}{3\Sigma_{a1}\Sigma_{a0}} \right] \ , \tag{17}$$

$$J(x) \equiv \int_{-1}^{1} \mu\psi(x,\mu) d\mu = -\frac{1}{3\Sigma_{a1}\Sigma_{a0}} \left[\frac{dq}{dx}(x) \right] \ . \tag{18}$$

Thus, even though $\psi(x,\mu)$ is quadratic in μ, Fick's Law is satisfied:

$$J(x) = -\frac{1}{3\Sigma_{a1}} \frac{d\phi}{dx}(x) \ . \tag{19}$$

Hence, for each $\psi(x,\mu)$ [Eq. (16)] driven by $q(x)$ [Eq. (12)], the corresponding $\phi(x)$ satisfies the conventional diffusion equation:

$$-\frac{1}{3\Sigma_{a1}} \frac{d^2\phi}{dx^2}(x) + \Sigma_{a0}\phi(x) = q(x) \ . \tag{20}$$

Eq. (16) holds for $\Sigma_{a0} \neq 0$. To obtain a bounded solution for $\Sigma_{a0} = 0$, one must scale certain of the constants q_j in Eq. (9) so that ψ remains bounded as $\Sigma_{a0} \to 0$. To accomplish this, we set:

$$q_1 = \Sigma_{a0}\beta_1 \ , \tag{21}$$

$$q_2 = \frac{3\Sigma_{a0}\Sigma_{a1}}{2}\left(\Sigma_{a0}\beta_0 - q_0\right) \ , \tag{22}$$

where β_0 and β_1 are arbitrary. Introducing Eqs. (21) and (22) into Eq. (16), we get

$$\psi(x,\mu) = \frac{\beta_0}{2} + \frac{\beta_1}{2}\left(x - \frac{\mu}{\Sigma_{a1}}\right) + \frac{3\Sigma_{a1}}{2}\left(\Sigma_{a0}\beta_0 - q_0\right)\left(\frac{x^2}{2} - \frac{\mu x}{\Sigma_{a1}} + \frac{3\mu^2 - 1}{3\Sigma_{a1}\Sigma_{a2}}\right) \ . \tag{23}$$

Letting $\Sigma_{a0} \to 0$, we obtain:

$$q(x) = q_0 \ , \tag{24}$$

$$\psi(x,\mu) = \frac{\beta_0}{2} + \left(x - \frac{\mu}{\Sigma_{a1}}\right)\frac{\beta_1}{2} - 3\left(\frac{\Sigma_{a1}x^2}{2} - \mu x + \frac{\mu^2 - 1/3}{\Sigma_{a2}}\right)\frac{q_0}{2} \ . \tag{25}$$

In Eq. (25), the coefficients of β_0 and β_1 are well-known solutions of the homogeneous $\Sigma_{a0} = 0$ transport equation with no absorption (Case, 1967). Also, the coefficients of q_0 represent a particular solution of the $\Sigma_{a0} = 0$ transport equation with a flat isotropic source. [For $\Sigma_{a0} = 0$, there exists no linear (or quadratic) flux for a spatially linear (or quadratic) source. However, such fluxes can be constructed that are cubic (or quartic) functions of x and μ.]

The angular flux in Eq. (25) has the following scalar flux and current:

$$\phi(x) = \beta_0 + \beta_1 x - \frac{3\Sigma_{a1}}{2} q_0 x^2 \ , \tag{26}$$

$$J(x) = q_0 x - \frac{\beta_1}{3\Sigma_{a1}} \ . \tag{27}$$

As before, these satisfy Fick's Law, and $\phi(x)$ satisfies the conventional diffusion equation with constant source q_0.

2.2 1-D Spherical Geometry

The above planar-geometry solutions can be used to construct fluxes and sources with 1-D spherical (or cylindrical) symmetry. To construct spherically symmetric solutions, we note that if x and μ in Eqs. (9) and (16) are replaced by y and η, or by z and ξ, one obtains 1-D solutions of Eq. (1) that very spatially in the y or z directions rather than the x-direction. Also, one can linearly combine these various fluxes and sources to obtain 3-D fluxes and sources that satisfy Eq. (1).

In particular, setting $q_1 = 0$ and adding the sources $q(x) + q(y) + q(z)$ and the fluxes $\psi(x,\mu) + \psi(y,\eta) + \psi(z,\xi)$, we obtain the 3-D source and angular flux:

$$q(\underline{r}) = 3q_0 + \left(x^2 + y^2 + z^2\right) q_2 \ , \tag{28}$$

$$\psi(\underline{r},\underline{\Omega}) = \frac{3q_0}{2\Sigma_{a0}} + \left[\left(x^2 + y^2 + z^2\right) - \frac{2}{\Sigma_{a1}}\left(\mu x + \eta y + \xi z\right) + \frac{2}{\Sigma_{a1}\Sigma_{a0}}\right]\frac{q_2}{2\Sigma_{a0}} \ , \tag{29}$$

which satisfy Eq. (1). [In Eq. (29), we used $\mu^2 + \eta^2 + \xi^2 = 1$.] This q and ψ have spherical symmetry. Introducing the familiar spherical-geometry spatial and angular variables

$$r \equiv \left(x^2+y^2+z^2\right)^{1/2} = |\underline{r}| \ , \tag{30}$$

$$\mu_s = \frac{\mu x+\eta y+\xi z}{(x^2+y^2+z^2)^{1/2}} = \frac{\underline{\Omega}\cdot\underline{r}}{|\underline{r}|} \ , \tag{31}$$

and replacing $3q_0$ by q_0, we obtain:

$$q(r) = q_0 + r^2 q_2 \ , \tag{32}$$

$$\psi(r,\mu_s) = \frac{q_0}{2\Sigma_{a0}} + \left(r^2 - \frac{2}{\Sigma_{a1}}r\mu_s + \frac{2}{\Sigma_{a1}\Sigma_{a0}}\right)\frac{q_2}{2\Sigma_{a0}} \ . \tag{33}$$

The corresponding scalar flux and current are:

$$\phi(r) = \int_{-1}^{1}\psi(r,\mu_s)d\mu_s = \frac{q_0}{\Sigma_{a0}} + \left(r^2 + \frac{2}{\Sigma_{a1}\Sigma_{a0}}\right)\frac{q_2}{\Sigma_{a0}} \ . \tag{34}$$

$$J(r) = \int_{-1}^{1}\mu_s\psi(r,\mu_s)d\mu_s = -\frac{2q_0 r}{3\Sigma_{a1}\Sigma_{a0}} \ . \tag{35}$$

As they must, these satisfy Fick's Law.

Eqs. (32) and (33) hold for $\Sigma_{a0} \neq 0$. To obtain a finite result for $\Sigma_{a0} = 0$, we scale q_2 via

$$q_2 = \frac{\Sigma_{a1}\Sigma_{a0}}{2}\left(\Sigma_{a0}\beta_0 - q_0\right) \ ; \tag{36}$$

then Eqs. (32) and (33) yield

$$q(r) = q_0 + \frac{\Sigma_{a1}\Sigma_{a0}}{2}\left(\Sigma_{a0}\beta_0 - q_0\right)r^2 \ , \tag{37}$$

$$\psi(r,\mu_s) = \frac{\beta_0}{2} + \left(r^2 - \frac{2}{\Sigma_{a1}}r\mu_s\right)\frac{\Sigma_{a1}}{4}\left(\Sigma_{a0}\beta_0 - q_0\right) \ . \tag{38}$$

Now letting $\Sigma_{a0} \rightarrow 0$, we obtain

$$q(r) = q_0 \ , \tag{39}$$

$$\psi(r,\mu_s) = \frac{\beta_0}{2} + \left(r\mu_s - \frac{\Sigma_{a1}r^2}{2}\right)\frac{q_0}{2} \ , \tag{40}$$

where β_0 is arbitrary. (In these equation, the coefficient of β_0 is the well-known "flat" solution of the sourceless $\Sigma_{a0} = 0$ transport equation. The coefficients of q_0 describe a particular solution of the $\Sigma_{a0} = 0$ spherical geometry transport equation with a spatially flat isotropic source.)

The scalar flux and current that correspond to $\psi(r,\mu_s)$ [Eq. (40)] are:

$$\phi(r) = \alpha_0 - \frac{\Sigma_{a1}q_0}{2}r^2 \ , \tag{41}$$

$$J(r) = \frac{rq_0}{3} \ . \tag{42}$$

Again, these satisfy Fick's Law.

2.3 1-D Cylindrical Geometry

Using the notation of Section 2.2, if we set $q_1 = 0$ and add the sources $q(x) + q(y)$ and fluxes $\psi(x,\mu) + \psi(y,\eta)$, we obtain 3-D sources and angular fluxes with 1-D cylindrical symmetry. We will not discuss these solutions further here.

3. PLANAR GEOMETRY DISCRETIZATION SCHEMES

Now we examine discrete-ordinates (S_N in angle, weighted-diamond in space discretizations of the planar geometry transport equation [Eq. (7)]. For simplicity, we assume isotropic scattering, $\Sigma_t = 1$, $\Sigma_s = c$, a spatial grid with cell edges $x_{j+1/2}$, and uniform cell width $h = x_{j+1/2} - x_{j-1/2}$. Integrating the S_N approximation to Eq. (7) over the j-th spatial cell $x_{j+1/2} \leq x \leq x_{j+1/2}$ and using the conventional notation for the cell-edge and cell-average fluxes (Lewis, 1984), we obtain the balance equation

$$\frac{\mu_n}{h}\left(\psi_{n,j+1/2} - \psi_{n,j-1/2}\right) + \psi_{n,j} = \frac{c}{2}\sum_{m=1}^{N}\psi_{m,j}w_m + \frac{Q_j}{2} \ , \tag{43}$$

with

$$Q_j \equiv \frac{1}{h}\int_{x_{j-1/2}}^{x_{j+1/2}} q(x)dx = q_0 + q_1 x_j + q_2\left(x_j^2 + \frac{h^2}{12}\right) \ . \tag{44}$$

To Eqs. (43), we append the “weighted diamond” auxiliary equations

$$\psi_{n,j} = \left(\frac{1+\alpha_n}{2}\right)\psi_{n,j+1/2} + \left(\frac{1-\alpha_n}{2}\right)\psi_{n,j-1/2} \ , \tag{45}$$

where α_n are the angular weights. These weights satisfy the constraints:

$$0 \leq \mu_n\alpha_n \leq |\mu_n| \quad \text{(stability)} \tag{46}$$

$$\mu_n = -\mu_m \quad \Rightarrow \quad \alpha_n = -\alpha_m \quad \text{(symmetry)} \ , \tag{47}$$

but otherwise are arbitrary. The Diamond Difference scheme results from specifying $\alpha_n = 0$. The Step Characteristic scheme results from specifying (Alcouffe, 1979):

$$\alpha_n = \alpha_n(h) = \frac{1+e^{-h/\mu_n}}{1-e^{-h/\mu_n}} - \frac{2\mu_n}{h} \ . \tag{48}$$

Eqs. (43)-(47) possess an exact solution with the same quadratic spatial behavior as the source. Thus, the cell-average and cell-edge fluxes have the form

$$\psi_{n,j} = f_{0,n} + f_{1,n}x_j + f_{2,n}\left(x_j^2 + \frac{h^2}{12}\right) \ , \tag{49}$$

$$\psi_{n,j+1/2} = g_{0,n} + g_{1,n}x_j + g_{2,n}x_j^2 \ , \tag{50}$$

with angle-dependent coefficients $f_{k,n}$ and $g_{k,n}$ to be determined. If the discrete solution were to “preserve” the analytic solution given by Eqs. (10) and (16), then $f_{k,n} = g_{k,n} = \psi_k(\mu_n)$ for for $0 \leq k \leq 2$ and $1 \leq n \leq N$. Unfortunately, we shall show that this is generally not the case.

Introducing Eqs. (49) and (50) into Eq. (43), using $x_{j\pm 1/2} = x_j \pm h/2$, and equating the coefficients of x_j^k for $k = 0, 1$, and 2, we obtain six algebraic equations for $f_{k,n}$ and $g_{k,n}$. These equations can be solved, first for $f_{2,n}$ and $g_{2,n}$, then for $f_{1,n}$ and $g_{1,n}$, and then for $f_{0,n}$ and $g_{0,n}$. Omitting the algebraic details, we obtain:

$$f_{2,n} = \frac{q_2}{2(1-c)} \ , \tag{51}$$

$$f_{1,n} = \frac{q_1}{2(1-c)} - \frac{q_2}{1-c}\mu_n \ , \tag{52}$$

$$\begin{aligned} f_{0,n} = \frac{q_0}{2(1-c)} - \frac{q_1}{2(1-c)}\mu_n + \frac{q_2}{1-c}\left[\frac{c}{3(1-c)} + \mu_n^2\right] \\ + \frac{q_2 h}{2(1-c)}\left[\frac{\rho c}{2(1-c)} + \mu_n \alpha_n\right] \ , \end{aligned} \tag{53}$$

where

$$\rho \equiv \frac{1}{2}\sum_{n=1}^{N} \mu_n \alpha_n w_n \ . \tag{54}$$

Also,

$$g_{2,n} = f_{2,n} \ , \tag{55}$$

$$g_{1,n} = f_{1,n} - h\alpha_n g_{2,n} \ , \tag{56}$$

$$g_{0,n} = f_{0,n} - \frac{h}{2}\alpha_n g_{1,n} + \frac{h^2}{3} g_{2,n} \ . \tag{57}$$

Introducing these results into Eqs. (49) and (50), we may calculate the cell-average scalar fluxes

$$\begin{aligned} \phi_j &\equiv \sum_{n=1}^{N} \psi_{n,j} w_n \\ &= \frac{q_0}{1-c} + \frac{q_1}{1-c}x_j + \frac{q_2}{1-c}\left[\left(x_j^2 + \frac{h^2}{12}\right) + \frac{1}{1-c}\left(\frac{2}{3} + h\rho\right)\right] \ , \end{aligned} \tag{58}$$

and the cell-edge currents

$$\begin{aligned} J_{j+1/2} &\equiv \sum_{n=1}^{N} \mu_n \psi_{n,j} w_n \\ &= -\frac{1}{1-c}\left(q_1 + 2q_2 x_{j+1/2}\right)\left(\frac{1}{3} + \frac{h\rho}{2}\right) \ . \end{aligned} \tag{59}$$

These quantities automatically satisfy the balance equation

$$\frac{1}{h}\left(J_{j+1/2} - J_{j-1/2}\right) + (1-c)\,\phi_j = Q_j \ . \tag{60}$$

By inspection, they also exactly satisfy

$$J_{j+1/2} = -\left(\frac{1}{3} + \frac{h\rho}{2}\right)\left(\frac{\phi_{j+1} - \phi_j}{h}\right) \ . \tag{61}$$

We now discuss these results.

1. In the limit $h \to 0$,

$$f_{k,n} = \psi_k(\mu_n) = g_{k,n} \ , \ 0 \le k \le 2 \ , \ 1 \le n \le N \ , \tag{62}$$

   where $\psi_k(\mu)$ is the coefficient of x^k in Eqs. (10) and (16). Thus, the correct solution is obtained in the fine (spatial) mesh limit.

2. For a constant source ($q_1 = q_2 = 0$), $f_{k,n} = \psi_k(\mu_n) = g_{k,n}$. Thus, as is well-known, all weighted diamond schemes preserve the infinite-medium "flat" solution.

3. For a linear source ($q_2 = 0$), one has for $k = 0$ and 1:

$$f_{k,n} = \psi_k(\mu_n) = g_{k,n} + (1-k)\frac{h}{2}\alpha_n f_{1,n} \ . \tag{63}$$

   Thus, the cell-average fluxes are preserved, but the cell-edge fluxes are not – unless $\alpha_n = 0$. The only weighted diamond scheme that preserves the "linear" infinite medium solution is the Diamond scheme, for which $\alpha_n = 0$.

4. For a quadratic source ($q_2 \neq 0$), no weighted diamond scheme preserves the complete angular flux. However, the Diamond solution preserves the correct cell-average scalar fluxes and cell-edge currents. No non-diamond scheme does this.

5. All discrete quadratic solutions constructed above satisfy the balance equation (60) and the Fick's Law (61). Eq. (61) contains the effective diffusion coefficient:

$$D(h) = \frac{1}{3} + \frac{h\rho(h)}{2} \ . \tag{64}$$

   The only weighted diamond scheme that has the correct (grid-independent) value of $D = 1/3$ is the Diamond scheme, for which $\rho(h) = 0$.

Previously, we showed that all analytic "quadratic" transport solutions satisfy the standard diffusion equation [Eq. (20)]. By using Eq. (61) to eliminate the currents from Eq. (60), we find that all the above discrete "quadratic" solutions satisfy the discrete diffusion equation

$$-\left(\frac{1}{3} + \frac{h\rho}{2}\right)\left(\frac{\phi_{j+1} - 2\phi_j + \phi_{j-1}}{h^2}\right) + (1-c)\phi_j = Q_j \ . \tag{65}$$

This discretization of the diffusion equation contains two types of truncation error:

1. The error associated with the finite-difference approximation

$$\frac{d^2\phi}{dx^2} \approx \frac{\phi_{j+1} - 2\phi_j + \phi_{j-1}}{h^2} \ ,$$

   which is a natural manifestation of the discretization process.

2. The error associated with the effective diffusion coefficient $D(h)$ [Eq. (64)].

The second error occurs for all non-diamond differencing schemes, for which $\rho > 0$. This error is an artifact that unphysically increases the flow of neutrons away from regions with high flux and into regions with low flux. Thus, it spatially "flattens" the solution. It has the potential to cause significant errors in the numerical estimates of the scalar flux for spatial grids with $h = O(1)$.

To show this, we plot in Figure 1 D versus h for the S_2 Diamond Difference (DD) and Step Characteristic (SC) schemes. For $h = 1$ mean free path, the SC diffusion coefficient is $D = 0.4128$, representing a 24% relative error. For $h = 2$, the SC diffusion coefficient is $D = 0.6147$, an 86% relative error. For large h, the error in the SC $D(h)$ grows nearly linearly with h.

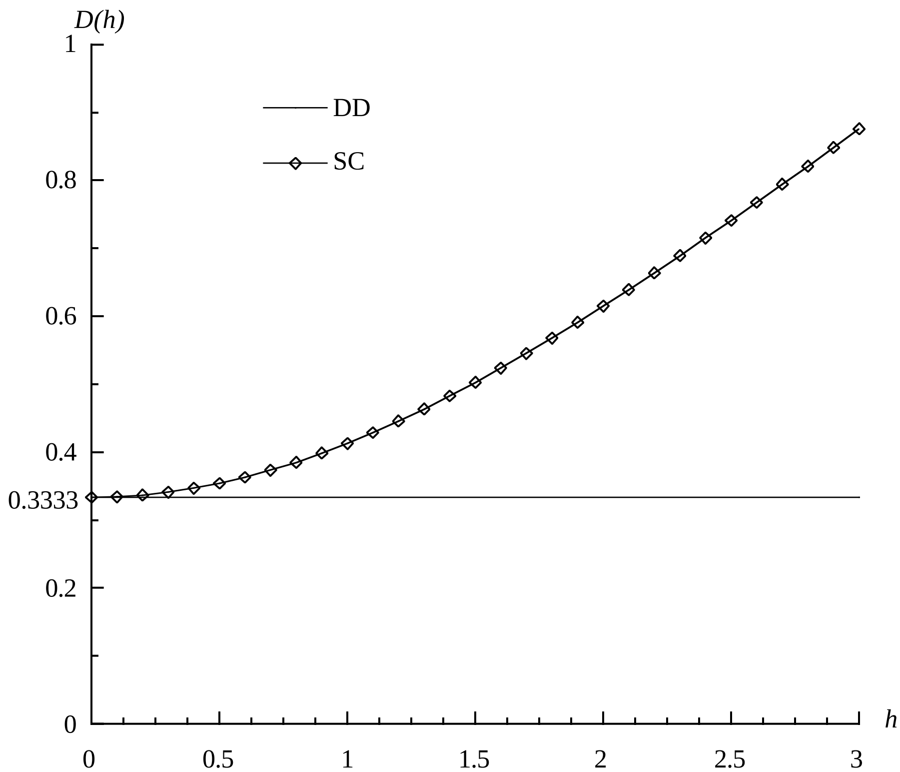

Fig 1: DD and SC Diffusion Coefficients

In Figure 2 we plot scalar fluxes for the following problem: a 20 mean free path thick slab, $c = 1$, reflecting left boundary, vacuum right boundary, driven by a constant source with magnitude chosen so that the exact S_2 scalar flux is unity at $x = 0$. The exact S_2 scalar fluxes are plotted, as are the DD and SC cell-average scalar fluxes, for $h = 1$ and 2 mean free paths.

For this problem, the DD scalar fluxes are extremely accurate, for both $h = 1$ and 2. However for these values of h, the SC scalar fluxes are inaccurate. For $h = 1$, the SC cell average scalar flux in the innermost cell is 0.8177, about an 18% error. For $h = 2$, the same flux is 0.5567, about a 44% error. The diffusion version of the given problem, solved with a diffusion coefficient that is 24% (86%) too large, yields a scalar flux that is low by the multiplicative factor $1/1.24 \approx .81$ $(1/1.86 \approx 0.54)$. These estimates agree very closely

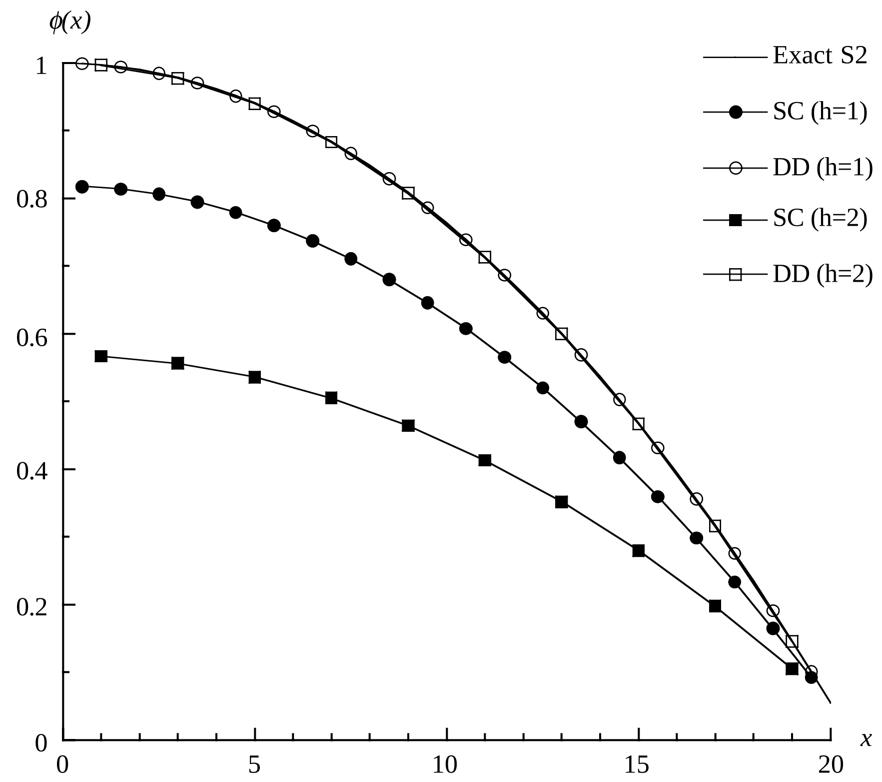

Fig 2: Exact and Approximate S_2 Scalar Fluxes

with the numerical results. (They do not perfectly agree because of the finite boundary at $x = 20$.)

These calculations show that among the class of weighted diamond schemes, the one scheme that preserves the "linear" transport solution – the Diamond Scheme – is the most accurate in diffusive problems - where locally, the physical angular flux behaves nearly linearly in space and angle. The preceding analysis explains why this happens: non-diamond schemes, which do not preserve the linear solution, have an unphysically large diffusion coefficient.

Next, we suggest a second possible use of the analytic quadratic infinite medium solutions constructed in Sec. 2. These "quadratic" angular fluxes all have scalar fluxes that satisfy the conventional diffusion equation. Thus, for finite-medium problems, if one solves the conventional diffusion equation – with boundary conditions that are perfectly consistent with the exact quadratic angular flux – one will obtain the exact scalar flux and current. However, it is easily shown that conventional Marshak, Mark, or other known boundary conditions are not consistent with an angularly quadratic angular flux! Thus, although the diffusion equation is capable of yielding the exact scalar fluxes, conventional boundary conditions will not permit this to happen. It is conceivable that by modifying the diffusion boundary conditions, one can robustly enable them to preserve the quadratic scalar fluxes generated in this paper, thereby yielding improvements in accuracy for other problems. However, this topic will not be discussed further here.

4. SPHERICAL GEOMETRY DISCRETIZATION SCHEMES

We now briefly discuss two subjects relevant to transport discretization schemes in spherical geometry.

First, the spherical geometry transport equation contains an angular derivative that must be discretized. Originally, the "diamond" angular differencing scheme

$$\psi_{n,j} = \frac{1}{2}\left(\psi_{n+1/2,j} + \psi_{n-1/2,j}\right) \tag{66}$$

was used in spherical geometry S_N codes. However, Morel proposed a "weighted-diamond" angular differencing scheme

$$\psi_{n,j} = \frac{1+\beta_n}{2}\psi_{n+1/2,j} + \frac{1-\beta_n}{2}\psi_{n-1/2,j} \ , \tag{67}$$

in which the weights β_n are uniquely chosen so that the angular flux can be a linear function of angle (Morel, 1984). [Eq. (66) does not permit $\psi_{n,j}$ to be linear in angle, because angular quadrature points μ_n do not generally lie midway between $\mu_{n-1/2}$ and $\mu_{n+1/2}$.] This modification significantly improves the accuracy of the resulting calculations, greatly reducing the erroneous "flux dip" at $r = 0$. In terms of the analysis in the present paper, we would say that Morel's modification enables the spherical geometry S_N equations to preserve the quadratic-in-space, linear-in-angle solutions given by Eqs. (32) and (33) (for $c < 1$), and (39) and (40) (for $c = 1$). The old "diamond" angular differencing [Eq. (66)] does not preserve these spherically-symmetric solutions.

Also, because the spherical geometry quadratic-in-space, linear-in-angle solutions are actually linear in angle – not quadratic, as in planar geometry – simple diffusion boundary conditions, such as the Marshak condition, will exactly preserve these solutions when used with the conventional diffusion equation. Thus, there may exist a simplicity in the spherical geometry diffusion boundary condition that is lacking in planar geometry!

5. DISCUSSION

We have constructed a family of infinite-medium solutions of the transport equation, consisting of angular fluxes that are linear (or quadratic) in space and angle, which are driven by sources that are linear (or quadratic) in space. These angular fluxes satisfy Fick's law; therefore their scalar fluxes satisfy the conventional diffusion equation.

Then, we investigated a certain class of transport discretization schemes and showed the following: schemes that preserve the "linear" infinite medium solution have a more accurate discrete form of Fick's law, and this leads to more accurate solutions for general diffusive problems, where Fick's law is relevant. [Another likely benefit is that the numerical solution should be less dependent on the spatial grid.] For these reasons, it is advantageous that a transport discretization scheme satisfies both the "linear" and "flat" infinite medium solutions.

Requiring a discretization scheme to preserve the "linear" infinite-medium transport solutions is more difficult to fulfill than requiring the scheme to preserve only the flat infinite-medium transport solutions. Even so, this is less difficult than requiring a scheme to preserve the exact solution in the absence of scattering – which certain characteristic methods are able to fulfill in planar geometry but not in other geometries (Knott, 1995), (Hong, 1998).

The analysis in this paper is relevant to the accuracy of transport discretization schemes applied to "diffusive" problems. An earlier *asymptotic* analysis has been successfully employed to address similar concerns (Larsen, 1992). The earlier asymptotic and the present analyses are complementary in several ways:

1. It is relatively easy to determine whether an S_N spatial differencing scheme preserves the linear solution on a structured or unstructured grid. However, the asymptotic analysis can be difficult to implement, particularly for multidimensional problems with unstructured grids (Adams, 1998), (Adams, 2001), (Wareing, 1999).

2. The asymptotic analysis has been developed mainly for radiative transfer problems in which spatial cells are optically thick. A different but related asymptotic analysis has been developed for neutron transport problems with spatial cells that are on the order of one mean free path in thickness, but this approach has received less attention (Larsen, 1987). The method developed in the present paper is (*i*) mathematically distinct from these asymptotic analyses, and (*ii*) applicable to all spatial grids, regardless of optical thickness.

3. When the asymptotic and the present analysis can be compared, they lead to the same conclusions.

We conjecture that a *necessary condition* for a transport discretization scheme to be accurate and robust in diffusive problems is that it preserves the linear transport solution. Unfortunately, this condition is *not sufficient* for problems with optically thick spatial cells. (The Diamond scheme preserves the linear solution, but instabilities interfere with the robustness of this scheme in optically thick grids.) However, it is possible that the "linearity" condition is both *necessary and sufficient* for common neutron transport schemes with spatial cells on the order of one mean free path in thickness.

To conclude, we note that in developing discretization methods for the diffusion equation, much emphasis has been placed on the ability of a (diffusion) discretization scheme to preserve the spatially "linear" solution (Kershaw, 1981), (Morel, 1992), (Morel, 1998), (Palmer, 2001). Experience and theory indicate that when the linear solution is preserved, numerical solutions of more general diffusion problems are more accurate and robust. The present paper suggests that the same principle should apply to the transport equation. The main complication with the transport equation is that "linear" solutions are linear in space *and* angle.

ACKNOWLEDGMENTS

I am grateful to Kord Smith and Marv Adams, for discussions at the ANS 2000 Winter meeting that prompted this work.

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