LA-UR--91-167

DE91 007399

Los Alamos National Laboratory is operated by the University of California for the United States Department of Energy under contract W-7405-ENG-36

TITLE INVESTIGATION OF LINEAR-DISCONTINUOUS ANGULAR DIFFERENCING FOR THE 1-D SPHERICAL-GEOMETRY S_N EQUATIONS

AUTHOR(S) W. F. Walters

J. E. Morel

SUBMITTED TO For publication in the proceedings of the ANS Pittsburgh 1991 International Topical Meeting on "Advances in Mathematics, Computations, and Reactor Physics," to be held April 28-May 1, 1991, in Greentree Marriott, Pittsburgh, PA

DISCLAIMER

Los Alamos Los Alamos National Laboratory
Los Alamos, New Mexico 87545

INVESTIGATION OF LINEAR-DISCONTINUOUS ANGULAR DIFFERENCING FOR THE 1-D SPHERICAL-GEOMETRY S_N EQUATIONS (U)

W. F. Walters and J. E. Morel
Los Alamos National Laboratory
Los Alamos, NM 87544

ABSTRACT

In this paper two new angular differencing schemes for use in spheres are derived and examined. These two schemes are the standard linear discontinuous (SLD) scheme and a hybrid scheme. In the hybrid scheme the angular flux is assumed to be quadratic and continuous in the angular cell whose boundary is the starting direction (μ = -1) and SLD in all other angular cells. The hybrid scheme is called the LDQ scheme. For smooth problems, both schemes are shown to exhibit fourth-order convergence as the angular mesh is refined while weighted-diamond (WD) and diamond-difference (DD) schemes are second order. For more difficult problems, all methods exhibit approximately second-order convergence, but the discontinuous schemes are always more accurate. The LDQ scheme is shown to have all the advantages of the SLD scheme while yielding in a more nearly isotropic flux at the center of the sphere Hence, the LDQ scheme should be the method of choice in problems where the WD and DD schemes are not sufficiently accurate.

Linear-discontinuous (LD) spatial differencing schemes for the S_N equations have been in use for many years, and their accuracy relative to other schemes has been well characterized.[1] However, LD angular differencing schemes have received very little attention. The schemes that have been developed treat several variables rather than the angular variables alone. For instance, Mordant[2] developed a space-angle LD scheme for the 2-D S_N equations in r-z geometry, and Honrubia and Aragones[3] developed a space-angle-energy LD scheme for the Fokker-Planck equation in 1-D spherical geometry. These studies focused upon the performance of each respective differencing scheme as a whole, i.e., as the entire multivariate mesh was refined. In contrast, the main purpose of our work is to investigate the accuracy of LD angular differencing when all but the angular mesh is fully refined. In addition, we address the treatment of highly anisotropic scattering in conjunction with an LD angular flux representation.

We have developed two angular differencing schemes for the 1-D spherical-geometry S_N equations. The first is a "standard" LD (SLD) scheme that represents a direct generalization of LD spatial schemes. The second is a hybrid LD/quadratic-continuous (LDQ) scheme which was developed in response to unexpected deficiencies in the SLD scheme. In this paper, the standard LD scheme is used for spatial differencing in all the codes used to generate results for comparing angular differencing schemes.

The derivation of the SLD scheme begins by first partitioning the angular domain into a set of N contiguous intervals $[\mu_{m-\frac{1}{2}}, \mu_{m+\frac{1}{2}}]$, with $\mu_{\frac{1}{2}} = -1$ and $\mu_{N+\frac{1}{2}} = 1$. Next we assume a linear-discontinuous dependence of the angular flux within each interval:

$$\psi(\mu) = \psi_m^+ \frac{\left[\mu - \mu_m^{(-)}\right]}{\left[\mu_m^{(+)} - \mu_m^{(-)}\right]} + \psi_m^{(-)} \frac{\left[\mu_m^{(+)} - \mu\right]}{\left[\mu_m^{(+)} - \mu_m^{(-)}\right]} \quad , \quad \mu_{m-\frac{1}{2}} < \mu \leq \mu_{m+\frac{1}{2}} \quad , \tag{1}$$

where $\mu_m^{\pm}$ denotes the local Gauss S_N quadrature points for the m'th angular interval, and $\psi_m^{\pm}$ denotes the angular flux at those points. We obtain two equations for the two unknowns in angular cell m by substituting from Eq. (1) into the transport equation, and taking the zero'th and first angular moments of the resulting equation, respectively. The local Gauss quadrature formula associated with the flux representation is used in conjunction with integration by parts to evaluate these moments exactly. The corresponding equations take the following form:

$$\begin{aligned} \frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2\left(\mu_m^{(+)}\psi_m^{(+)} + \mu_m^{(-)}\psi_m^{(-)}\right)\right] w_m + \frac{1}{r}\left[\left(1-\mu_{m+\frac{1}{2}}^2\right)\psi_{m+\frac{1}{2}} - (1-\mu_{m-\frac{1}{2}}^2)\psi_{m-\frac{1}{2}}\right] \\ + \sigma_t\left[\psi_m^{(+)} + \psi_m^{(-)}\right] w_m = \left[Q_m^{(+)} + Q_m^{(-)}\right] w_m \quad , \end{aligned} \tag{2}$$

and

$$\begin{aligned} &\frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2\left(\mu_m^{(+)}\psi_m^{(+)} + \mu_m^{(-)^2}\psi_m^{(-)}\right)\right] w_m \\ &+ \frac{1}{r}\left[\mu_{m+\frac{1}{2}}(1-\mu_{m+\frac{1}{2}}^2)\psi_{m+\frac{1}{2}} - \mu_{m-\frac{1}{2}}(1-\mu_{m-\frac{1}{2}}^2)\psi_{m-\frac{1}{2}}\right] \\ &- \frac{1}{r}\left[\left(1-\mu_m^{(+)^2}\right)\psi_m^{(+)} + \left(1-\mu_m^{(-)^2}\right)\psi_m^{(-)}\right] w_m \\ &+ \sigma_t\left[\mu_m^{(+)}\psi_m^{(+)} + \mu_m^{(-)}\psi_m^{(-)}\right] w_m \\ &= \left[\mu_m^{(+)}Q_m^{(+)} + \mu_m^{(-)}Q_m^{(-)}\right] w_m \quad . \end{aligned} \tag{3}$$

where $\psi_{m-\frac{1}{2}}$ is known from initial conditions, and $\psi_{m+\frac{1}{2}}$ is defined in terms of $\psi_m^{(-)}$ and $\psi_m^{(+)}$ by Eq. (1). The two equations for each cell are solved simultaneously, beginning with the equations for the first cell. The solution for cell m provides the initial flux for cell m + 1. However, note that an initial flux value is not needed for the first cell. Thus, the SLD scheme does not require the calculation of a starting-direction flux.

Computational testing indicates that SLD scheme gives high-order accuracy for simple problems with smooth solutions. However, for certain classes of problems and quadrature orders, the SLD scheme can be considerably less accurate than the diamond-difference (DD) scheme. This deficiency arises from the fact that the starting direction flux, which does not appear in the SLD scheme, strongly contributes to the accuracy of the DD scheme near the origin. To compensate for this flaw, we have developed a hybrid scheme which

uses a quadratic-continuous scheme in the first angular cell and the SLD scheme in all other cells. The unknowns in the first cell are the angular fluxes at the three local Radau quadrature points, the first of which is $\mu = -1$. The flux along this direction corresponds to the starting-direction flux, and is obtained by solving the slab-geometry equation at $\mu = -1$. Equations for the two other fluxes in the cell are obtained by using the local Radau quadrature formula to obtain zero'th and first moment equations. The quadrature formula is exact for this purpose. Note that the starting-direction flux is weighted in the LDQ scheme, whereas it is always unweighted in standard angular differencing schemes. Thus, the LDQ scheme effectively gives rise to an asymmetric quadrature set. An obvious way to eliminate this asymmetry is to use a quadratic-continuous scheme in both the first and last cells, but this scheme gives very inaccurate solutions in certain types of problems.

To clarify this point, let us consider the form of the starting-direction equation used for spheres

$$\mu\frac{\partial\psi}{\partial r} + \frac{(1-\mu^2)}{r}\frac{\partial\psi}{\partial r} + \sigma\psi = Q \tag{4}$$

Normally we set μ=-1 in this equation and solve the slab starting-direction equation in which the second term in Eq. (4) is zero. If the angular flux contains a delta function in μ at -1, then this term can not be set to zero, and a simple slab starting-direction equation can not be obtained. Normally the angular flux near μ=-1 is a smooth function, and there is no problem.

Now to generate a symmetric quadrature set, one could solve a finishing-direction equation obtained by setting μ=+1 in Eq. (4). There is a problem with doing this! The angular flux from a point source in a vacuum exhibits delta function behavior at μ=+1, and the second term in Eq. (4) can not be set to zero. If this term were set to zero for this problem, then the finishing-flux would not fall off as $1/r^2$ as it should; and in fact, the angular flux at μ=+1 would be a constant at all points! This is the reason an asymmetric set is used, and a finishing-direction equation is not solved. The angular flux at μ=+1 is determined from the linear relation in the angular interval bordering μ=+1. The flux is thus not pinned at μ=+1.

Using the transport equation, it is easy to show that the angular flux at the center of a sphere should be isotropic and equal to the starting direction value. At the center of the sphere, the LD scheme used in the spatial differencing computes the angular flux for all incoming directions and *does not assume that the value for all the incoming directions is fixed at the starting direction value* as some other methods do. At the center of the sphere, the agreement between the value of the angular flux at the starting direction and the values of the angular flux for all other incoming discrete directions is then a measure of the accuracy of the method.

In Fig. 1 we show the results from a simple test problem which clearly demonstrates the superiority of the LDQ method. In this problem the only source is assumed to be an isotropic boundary source at the surface of a homogeneous purely-absorbing sphere. That is, all incoming directions have the same amplitude at the surface. The problem is examined using an S_4 quadrature set so there are two incoming directions for all the schemes except the LDQ scheme which has three incoming directions because of the inclusion of the starting direction. Clearly, the WD and LDQ schemes yield an angular flux that is more nearly isotropic at the center of the sphere as compared to the SLD scheme. The values of the angular flux at the two incoming directions in the SLD scheme are nearly equal but they vary considerably from the starting direction value of 3.64. This purely-absorbing test problem is used because it is the most difficult test of the isotropic flux condition at

sphere center. Scattering tends to smooth out the flux, and it is difficult to discern the relative accuracy of the various angular differencing schemes.

In order to treat highly anisotropic scattering, we have developed Galerkin quadratures[4] for the SLD and LDQ schemes. These quadratures were tested on electron transport calculations and gave very accurate solutions.

We have performed a series of calculations to compare the accuracy of our schemes with that of the DD scheme and the weighted-diamond (WD) scheme of Morel and Montry.[5] All of these calculations were performed for the same problem: a homogeneous purely-absorbing sphere with an absorption cross section of 1 cm^{-1}, a radius of 1 cm, a constant isotropic distributed source, and a vacuum condition at the outer surface. Standard linear-discontinuous spatial differencing was used with 1000 cells in all of the calculations to ensure spatial convergence. The errors in the global particle leakage from the sphere are compared for the various schemes in Table 1. Both the SLD and LDQ schemes give essentially fourth-order accuracy for this problem, while the DD and WD schemes give essentially second-order accuracy. It is conjectured that these high orders of convergence are obtained for two reasons. First, the angular flux is extremely smooth in this problem. Second, an integral quantity is being examined.

To test this conjecture, a third test problem is examined. This is a 5 cm radius purely absorbing sphere with an absorption cross section of 1 cm^{-1} with a point source at the center. The angular flux in this problem is not at all smooth. Analytically, all of the angular flux is concentrated in the μ=+1 direction. That is a delta function at μ=+1. The numerical results for net leakage at the surface and the scalar flux at the surface are shown in Figs. 2 and 3 along with the exact analytical result. The LDQ and the SLD schemes give the same result because the starting-direction flux is not involved in the calculation. WD/DSN is the weighted diamond in angle using double Gauss quadrature. WD/SN is the weighted diamond in angle using Gauss quadrature. The spatial mesh is very fine for all runs; it is 1000 meshes per mean free path. In both cases the discontinuous method is seen to be more accurate. It is clear that the LDQ/SLD results are more accurate than the WD/SN and WD/DSN results. The Gauss results are much more accurate than the double Gauss results because the Gauss set always has a point nearer to +1 than the double Gauss set ast the same SN order. The discontinuous scheme fairs well in this problem, in spite of employing equal μ intervals and having no points near +1, simply because there are two degrees of freedom in each interval including the one bordering μ=+1. For the LDQ, WD/DSN, and WD/SN results, the order of convergence for the leakage is 1.95, 1.68, and 1.83, respectively. For the angular flux at the surface (5 cm), these orders of convergence are 2.2, 1.68, and 1.83, respectively. Thus, the prior conjecture is true; the fourth-order convergence of the previous test problem is not observed in this problem. The order of convergence here is approximately 2.0. Notice that the discontinuous result tends to reach the asympotic limit at a lower S_N order than do the two weighted diamond results.

In all cases studies, the accuracy of the LDQ scheme was found to be equal to or superior to that of the diamond or weighted diamond schemes. For most problems the WD and DD schemes could be sufficient. For classes of problems where this is not true, the LDQ scheme is now an alternative. No attempt has been made to optimize the coding for these discontinuous schemes. These schemes are really bilinear space-angle schemes with four unknowns per space-angle cell.

REFERENCES

1. R. E. Alcouffe, E. W. Larsen, W. F. Miller, Jr., and B. R. Wienke, **Nucl. Sci. Eng.**, 71, 11 (1979).

2. M. Mordant, **Nucl. Sci. Eng.**, 92, 218 (1986).

3. J. J. Honrubia and J. M. Aragones, **Nucl. Sci. Eng.**, 92, 98 (1986).

4. J. E. Morel, **Nucl. Sci. Eng.**, 101, 72 (1989).

5. J. E. Morel and G. R. Montry, **Transport Theory and Statistical Physics**, 13, 615 (1984).

TABLE 1. Computational Results

Method	Quadrature Order	Error	Order Accuracy
LDQ	8	3.024×10^{-4}	-
LDQ	16	1.496×10^{-5}	4.3
LDQ	32	8.764×10^{-7}	4.1
SLD	8	3.195×10^{-4}	-
SLD	16	1.532×10^{-5}	4.4
SLD	32	8.664×10^{-7}	4.1
DD	8	9.868×10^{-4}	-
DD	16	2.951×10^{-4}	1.7
DD	32	7.886×10^{-5}	1.9
WD	8	9.722×10^{-4}	-
WD	16	2.940×10^{-4}	1.7
WD	32	7.885×10^{-5}	1.9

Fig. 1. Angular Flux at r=0.0 for Incoming Directions.

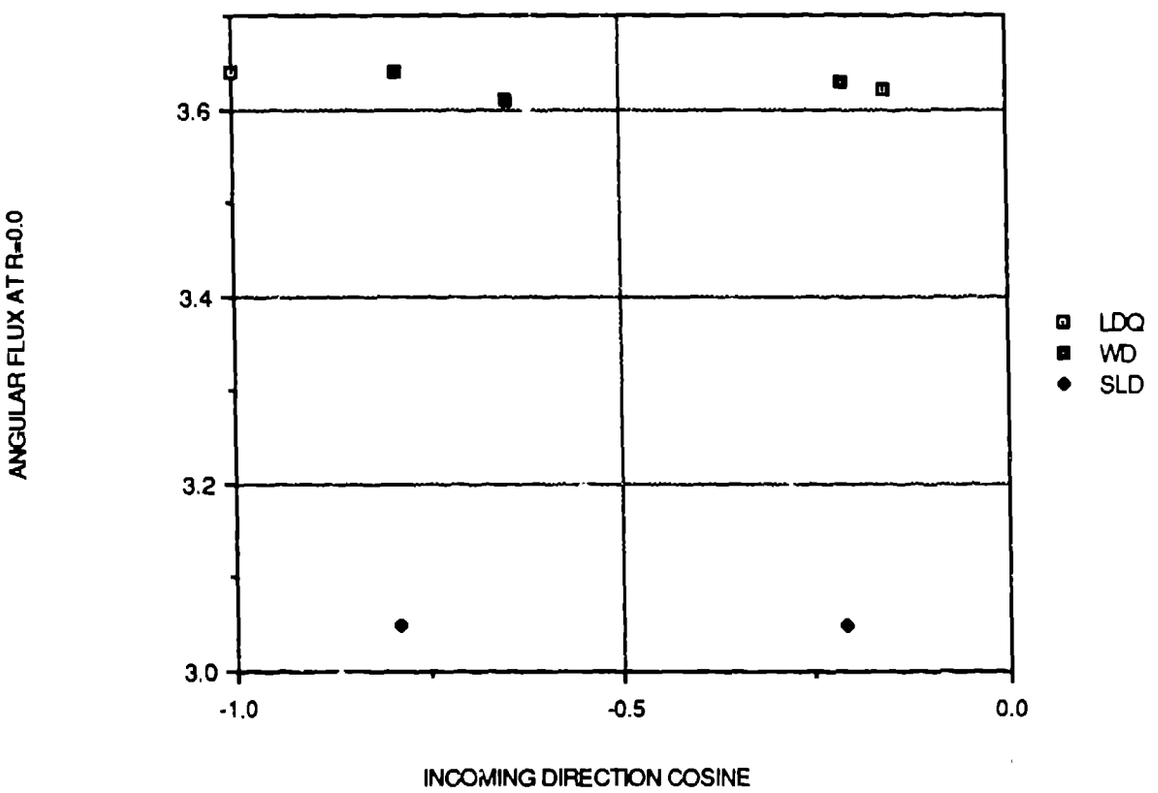

Fig. 2. Leakage vs S_N Order.

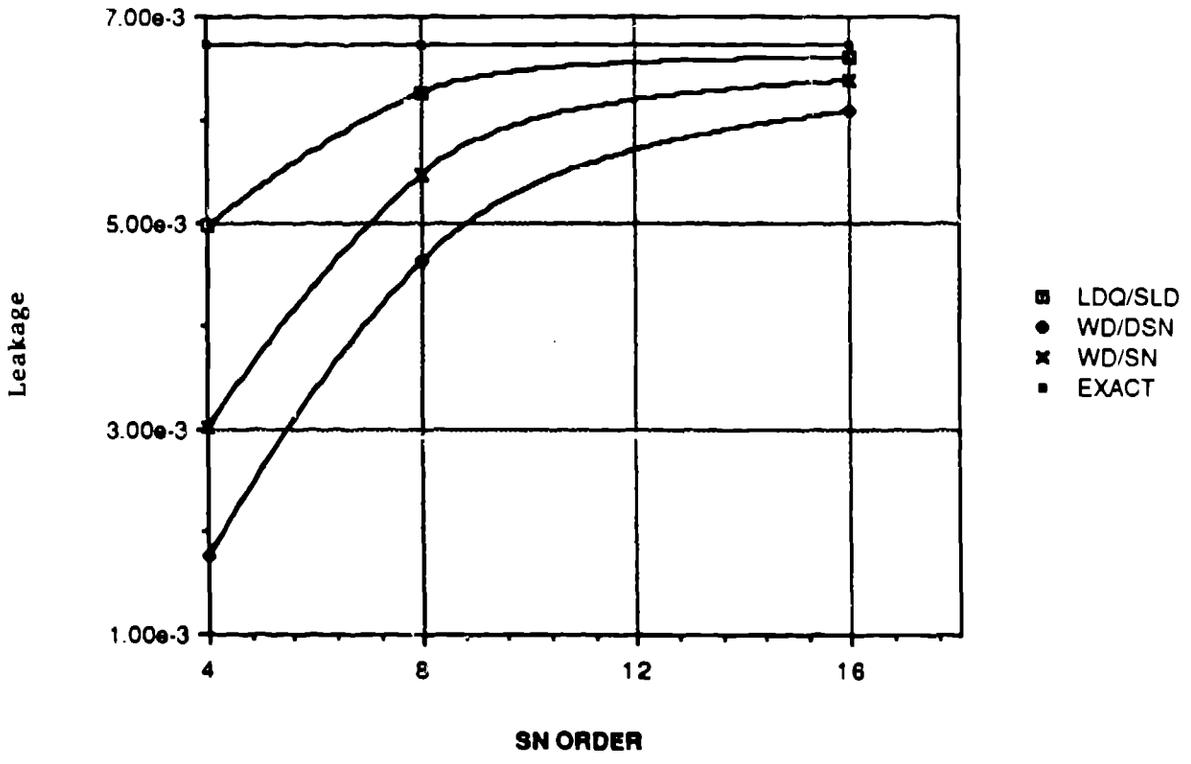

Fig. 3. Scalar Flux at Surface vs S_N Order.