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TITLE: AUGMENTED WEIGHTED DIAMOND FORM OF THE LINEAR NODAL SCHEME FOR CARTESIAN COORDINATE SYSTEMS

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AUGMENTED WEIGHTED DIAMOND FORM OF THE LINEAR NODAL SCHEME FOR CARTESIAN COORDINATE SYSTEMS

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ABSTRACT

The equations of the high order linear nodal numerical scheme are cast in an augmented weighted difference form for three dimensional cartesian nodes. The coupling exhibited by these equations indicate that this new algorithm is simpler and hence faster than previous nodal schemes of this degree of accuracy. A well-logging problem and a fast reactor problem are examined. The new scheme developed here is compared with the classical linear-linear nodal scheme and the diamond difference scheme. For the well-logging problem, it is found that the new scheme is both faster and simpler than the classical linear-linear nodal scheme while sacrificing little in accuracy. Even though the new scheme is more accurate than the diamond difference scheme for the reactor problem, the results indicate that state of the art acceleration methods are needed for nodal schemes.

INTRODUCTION

Two high order nodal schemes used to solve the discrete-ordinate form of the transport equation for two dimensional Cartesian systems have been developed by this author. These are the linear-linear (LL) scheme described in detail in Ref. 1, and the linear nodal (LN) scheme sketched briefly in Ref(s). 2 and 3. Both of these schemes assume a linear source expansion in each node and a linear representation of the angular flux on the node faces. This paper contains several new and significant results. First, the LN equations are derived in detail for the three dimensional Cartesian system. Second, these equations are cast in an augmented weighted diamond difference form. Third, the equations are reduced to the two dimensional form and two problems are investigated. A well logging problem is investigated using both the original LL scheme and this new formulation of the LN scheme. The second problem is a fast reactor benchmark problem which is examined using the LN scheme and the standard diamond difference (DD) scheme. For the well logging problem, it is found that this formulation of the LN scheme is much less complex, hence faster, than the LL scheme while

exhibiting only a slight degradation in accuracy. In the fast reactor problem, the LN scheme is once again found to be superior to the DD scheme but not by as great a degree as found in another fast reactor problem analyzed in Ref. 3.

Recently two papers pertaining to the nodal method in neutron transport have appeared in the literature. In Ref. 4 an augmented weighted diamond scheme is indicated for the low order constant-linear (CL) nodal scheme. The authors note however that significant improvement over the CL scheme is obtained using the LL scheme. In Ref. 5 a direct extension of the two dimensional LL equations derived in Ref. 1 to three dimensions is presented. In three dimensions, it is correctly noted that a system of nine fully coupled simultaneous equations must be solved for each discrete ordinate for each node. The equations developed here exhibit the high order accuracy of the full LL scheme while retaining the speed and simplicity inherent in an augmented weighted diamond form. An additional benefit is that these equations can be solved easily for the case of a voided node while the equations of the LL scheme and the original formulation of the LN scheme constitute a singular system for this case. Explicit relations are derived for the weight functions.

I. DEVELOPMENT OF EQUATIONS

Define the node i,j,k to be the rectangular parallelepiped bounded by $x_L \le x \le x_R$, $y_{BM} \le y \le y_T$, $z_{BK} \le z \le z_F$ with $\Delta x = x_R - x_L$, $\Delta y = y_T - y_{BM}$, $\Delta z = z_F - z_{BK}$, $\bar{x} = (x_L + x_R)/2$, $\bar{y} = (y_T + y_{BM})/2$, and $\bar{z} = (z_F + z_{BK})/2$.

Throughout this summary L, R, BM, T, BK, F, and A are subscripts such that L = left, R = right, BM = bottom, T = top, BK = back, F = front, and A = average. The subscripts x, y, and z indicate moments of a quantity with respect to that coordinate. ψ and φ are neutron angular fluxes. ψ is the first moment of the angular flux on a face of the node. The discrete-ordinates form of the transport equation for direction m and energy group g is

$$\mu_m \partial\psi_{m,g}(x,y,z)/\partial x + \eta_m \partial\psi_{m,g}(x,y,z)/\partial y + \xi_m \partial\psi_{m,g}(x,y,z)/\partial z + \sigma_g \varphi_{m,g}(x,y,z) = s_{m,g}(x,y,z) \quad . \tag{1}$$

Hereafter the subscripts m and g will be suppressed. σ is the neutron total cross-section. S is the source driving the transport equation. μ, η, and ξ are the x- y- and z- direction cosines. For simplicity in developing the equations of the LN scheme, it will be assumed that $\mu, \eta, \xi > 0$. That is, the neutron flow is from left to right, bottom to top, and back to front. The nodal equations for the x coordinate only will be indicated.

Using the neutron balance equation and the first x-moment balance equation; the first nodal equation for ψ_R, the angular flux on the right face, is

$$\psi_R = \psi_L \exp(-\tau_x) + P0(\tau_x) \cdot \left[\varepsilon_x \psi_A + \psi_R - \psi_L \right] + \left[2P1(\tau_x) - P0(\tau_x) \right] \cdot \left[3 \cdot (\psi_R + \psi_L - 2\psi_A)/\tau_x + \psi_x \right] \quad . \tag{2}$$

Here ψ_x is the node average x-moment which appears in the first x-moment balance equation. Additionally,

$$P0(\tau_x) = \frac{\left[1 - \exp(-\tau_x) \right]}{\tau_x} \quad , \qquad P1(\tau_x) = \frac{\left[1 - P0(\tau_x) \right]}{\tau_x} \quad ,$$

and

$$\tau_x = \sigma \Delta x / \mu \quad . \tag{3}$$

The second nodal equations for θ_{Tx}, the x-moment of the angular flux on the top face, and θ_{Fx}, the x-moment of the angular flux on the front face, are

$$\theta_{Tx} = \theta_{BMx} \exp(-\tau_y) + P0(\tau_y) \cdot \left[\varepsilon_y \psi_x + (\theta_{Tx} - \theta_{BMx}) \right] + \left[2P1(\tau_y) - P0(\tau_y) \right] \cdot \left[3 \cdot (\tau_y/\tau_x) \cdot (2\psi_y - \theta_{Ry} - \theta_{Ly}) \right] \quad , \tag{4}$$

and

$$\theta_{Fx} = \theta_{BKx} \exp(-\tau_z) + P0(\tau_z) \cdot \left[\varepsilon_z \psi_y + (\theta_{Fx} - \theta_{BKx}) \right] +$$

$$[2P1(\epsilon_z) - P0(\epsilon_z)] + [3 \cdot (\epsilon_z/\epsilon_x) \cdot (2\psi_z - \theta_{Rz} - \theta_{Lz})] \quad . \qquad (3b)$$

At this point these equations are exactly the linear-linear nodal equations. That is, linear expansions have been assumed for the source and the angular fluxes on the surface of the node. The linear nodal scheme is arrived at by assuming the diamond relation in only the last term of (3a) and (3b . That is,

$$\psi_y = (\theta_{Ry} + \theta_{Ly})/2 \text{ , and } \psi_z = (\theta_{Rz} + \theta_{Lz})/2 \quad .$$

Now (3a) and (3b) can be solved for ψ_x to yield,

$$\psi_x = \theta_{Tx} \cdot [P1(\epsilon_y)/P0(\epsilon_y)] + \theta_{BKx} \cdot [1 - P1(\epsilon_y)/P0(\epsilon_y)] \text{ , and} \qquad (4a)$$

$$\psi_x = \theta_{Fx} \cdot [P1(\epsilon_z)/P0(\epsilon_z)] + \theta_{BKx} \cdot [1 - P1(\epsilon_z)/P0(\epsilon_z)] \quad . \qquad (4b)$$

In the limit of small Δy (4a) becomes the diamond relation, and in the limit of small Δz (4b) becomes the diamond relation. In the limit of large Δy and Δz these relations become the step relations,

$$\psi_x = \theta_{Tx} \text{ , and } \psi_x = \theta_{Fx} \quad .$$

The x-moment balance equation containing ψ_x is

$$3 \cdot [\psi_R + \psi_L - 2\psi_A] + (\epsilon_x/\epsilon_y) \cdot (\theta_{Tx} - \theta_{BKx}) + (\epsilon_x/\epsilon_z) \cdot (\theta_{Fx} - \theta_{BKx}) +$$

$$\epsilon_x\psi_x = S\Delta x/\mu \quad . \qquad (5)$$

Now (4a) and (4b) can be used in (5) and ψ_x can be determined as a function of ψ_A, ψ_R, ψ_L, inflow quantities, the source and its moment. Specifically

$$\psi_x = [3 \cdot (2\psi_A - \psi_L - \psi_R) + (\rho_y\theta_{BKx} + \rho_z\theta_{BKx} + S_x) \cdot \Delta x/\mu] /$$

$$[\epsilon_x + (\rho_y + \rho_z) \cdot \Delta x/\mu] \quad , \qquad (6)$$

where

$$\rho_y = [\ P0(\epsilon_y)/\ P1(\epsilon_y)\ ] \cdot \eta/\Delta y, \text{ and } \rho_z = [\ P0(\epsilon_z)/\ P1(\epsilon_z)\ ] \cdot \xi/\Delta z \quad .$$

If the expression for ψ_x given by (6) is substituted into (2), the augmented weighted diamond form is obtained.

$$\psi_A = (\ 1 - \alpha_x\ ) \cdot \psi_L/2 + (\ 1 + \alpha_x\ ) \cdot \psi_R/2 - F_x\epsilon_x(\Delta x/\mu)$$

$$[\ \rho_y\theta_{BMx} + \rho_z\theta_{BKx} + S_x\ ] \quad , \tag{7a}$$

where

$$\alpha_x = F_x \cdot (\rho_y + \rho_z + \epsilon_x) \quad . \tag{7b}$$

$$F_x = [P2(\epsilon_x) - P1(\epsilon_x)] / [(\rho_y + \rho_z) \cdot (P1(\epsilon_x) + 2P3(\epsilon_x) - 3P2(\epsilon_x)] -$$

$$P0(\epsilon_x)] \quad , \tag{7c}$$

$$P2(\epsilon_x) = [1 - 2P1(\epsilon_x)] / \epsilon_x \quad , \text{ and}$$

$$P3(\epsilon_x) = [1 - 3P2(\epsilon_x)] / \epsilon_x \quad .$$

Now the augmented diamond relation (7a) and its y- and z-coordinate analogs can be used to determine the outflow fluxes as a function of the average flux. Substituting these relations into the neutron balance equation, the average angular neutron flux ψ_A can be determined. Extrapolations can then be performed to obtain the outflow angular fluxes. Knowing these quantities ψ_x, ψ_y, and ψ_z can be determined from (6) and its y- and z-coordinate analogs. The outflow values of θ can be determined by extrapolation using (4a), (4b) and their y- and z-coordinate analogs.

This completes the derivation of the augmented weighted form of the LN equations. Notice that the two-dimensional form of these equations can be obtained by simply setting $\Delta z = \infty$ which implies that $\rho_z = 0$.

II. IMPLEMENTATION

To obtain expressions for α_x, F_x, ρ_x, and ρ_z that are accurate, fast, and retain the correct behavior for both large and small values of ϵ_x, ϵ_y and ϵ_z; the Pade'(2,3) approximation for the exponent

$$\exp(\epsilon) = (60 - 24\epsilon + 3\epsilon^2)/(60 + 36\epsilon + 9\epsilon^2 + \epsilon^3) \qquad (8)$$

is used. The Pade' approximation is positive for all real values of ϵ and has the correct limits for $\epsilon \to 0$ and $\epsilon \to \infty$. Using this relation ρ_x and ρ_z are found to be ratios of polynomials in either ϵ_x or ϵ_z. Assuming that the ρ's are known then F_x is a ratio of polynomials in ϵ_x. The α_x weights then contain only powers of ϵ_x, ϵ_y and ϵ_z .

The coding for this new form of the LN scheme has been placed in the TWOTRAN-II code.[6] The coding has not been updated in any way to take advantage of the vector processing available on the CRAY 1 machine. In addition the coarse mesh rebalance inner iteration acceleration and group collapsed outer rebalance acceleration of the host TWOTRAN-II code have been retained.

There is no negative flux fixup employed in the inner sweeping loop of the code at all. After all the ordinate directions have been scanned in an inner iteration and the scalar flux ϕ and its spatial moments ϕ_x and ϕ_y have been computed, the moments ϕ_x and ϕ_y are "rotated" to ensure that the linear representation of the scalar flux is positive everywhere in the node. The value of the average scalar flux in the node is not changed in any way. This "rotation" seems to work well and does not impact the running time since it is in the outer loop.

III. RESULTS AND CONCLUSIONS

The results of an analysis of a two-dimensional well logging problem investigated in Ref. 7 are shown in Fig. 1. The absorptions are those occurring in the detector of a well logging tool. The minimum value of the mean free path in this problem is .67 cm. This means that a node size of 5 cm. is roughly 1/ mean free paths. It should not be surprising then that the diamond difference solution is so ill behaved at this node size. There are so many negative flux fixups that the result is almost meaningless. At

a node size of 2 cm. or 3 mean free paths both the LN and the LL solutions are well within one percent of the reference extrapolated value for detector absorption. The LN and LL values of absorption differ by only .1 percent at this node size. Practically speaking then, these two schemes yield the same answer if one percent accuracy is desired.

The second problem to be examined is the SNR 300 fast reactor benchmark model.[8] A comparison of K_{eff} eigenvalues determined with the DD scheme as found in the TWODANT code with those obtained using the LN scheme and the new algorithm as implemented in TWOTRAN-II are shown. The results are somewhat surprising. As expected, the LN results are more accurate for a given mesh than the DD eigenvalue. The diamond scheme requires four times as many nodes to generate an eigenvalue as accurate as that determined with the LN scheme. In Ref. 3 it was found that the DD scheme required between 9 and 16 times as many nodes to generate an eigenvalue as accurate as that determined with the LN scheme. The current problem appears to be more diffusion like with a maximum coarse mesh finer (in terms of mean free path) than that associated with the ZPPR 7a analyzed in Ref. 3. For this type of problem, it is apparent that the TWODANT code using its state of the art acceleration methods for the DD scheme can only be challenged by a state of the art LN code using similar acceleration methods.

In two dimensions the LL scheme requires the solution of four simultaneous equations in four unknowns followed by the solution of three explicit equations. On the other hand, the LN scheme requires the solution of seven explicit equations four of which are simple extrapolations. In three dimensions the comparison is even more stunning. The LL scheme requires the solution of nine simultaneous equations in nine unknowns followed by the solution of four explicit equations. The LN schemes requires the solution of thirteen explicit equations, nine of which are simple extrapolations. It should be clear that the LN scheme is preferable due to its simplicity and speed as compared to the LL scheme.

Speed is, of course, dependent upon the exact coding used. If weight functions are precomputed and stored, the maximum speed is attained but a storage penalty is paid. The storage required is the size of the coarse mesh times the number of ordinates in an octant (three dimensions). The weights were not precomputed and stored in the current test code.

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TABLE I

SNR 300 TWO DIMENSIONAL XY BENCHMARK (CONVERGENCE CRITERION = 10^{-4})

Mesh	K_{eff} Diamond Difference (TWODANT)	K_{eff} Linear Nodal
19 X 19	1.1159	1.1167
38 x 38	1.1169	1.1172
76 x 76	1.1172	-
152 x 152	1.1173	-

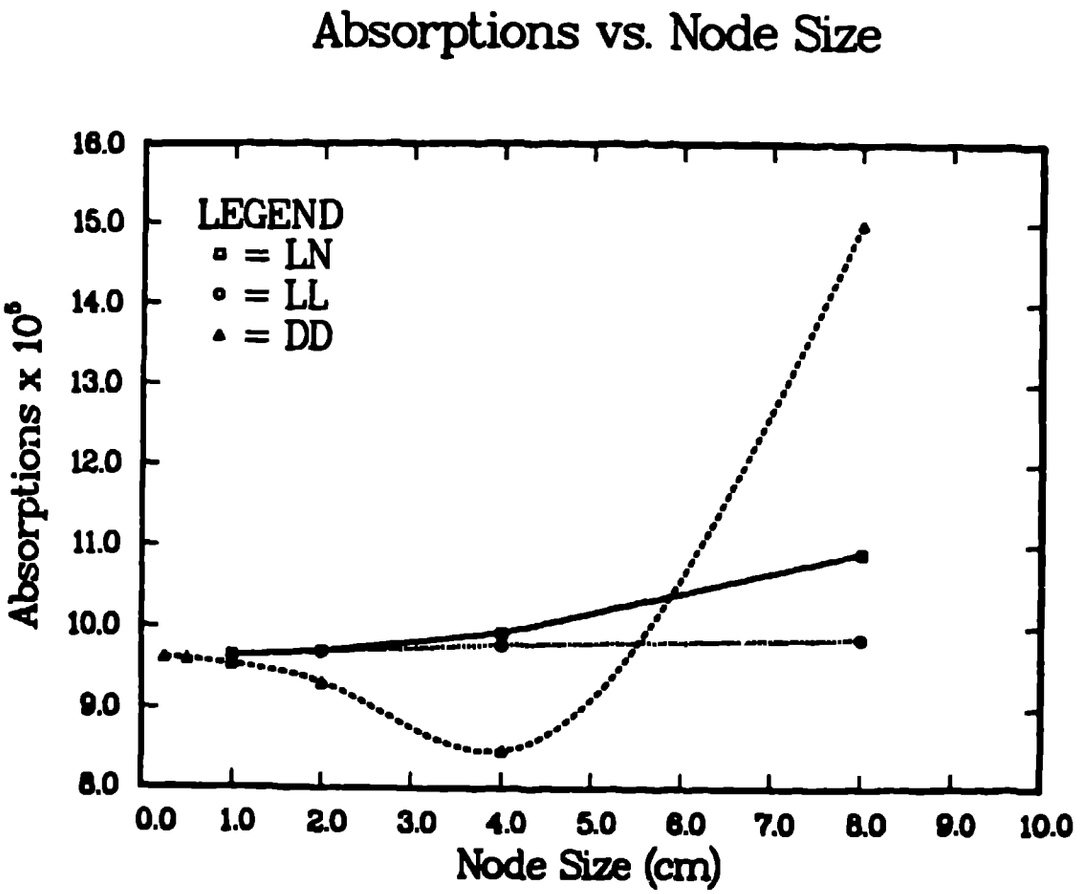

Fig. 1