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A NONLINEAR POSITIVE METHOD FOR SOLVING THE TRANSPORT EQUATION ON COURSE MESHES

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ABSTRACT

A new nonlinear S_n transport differencing scheme for slab geometry is presented that is fourth order accurate for small meshes and is strictly positive. The new scheme has been coded into the existing ONELD code and tested. We present numerical results to demonstrate the accuracy and positivity of this new scheme.

I. INTRODUCTION

Since the inception of the discrete ordinates (S_n) angular treatment of the transport equation, code developers have tried to develop accurate and positive spatial differencing schemes to solve the S_n equations. One of the first differencing scheme used was the simple step or constant discontinuous method[1]. The scheme is strictly positive but only first order accurate in terms of spatial errors, and therefore; deemed too inaccurate for practical use. The diamond difference method[1] (DD) has been used for many years because it is second order accurate for small meshes. However, the DD method can result in negative fluxes in one dimensional problems for meshes thicker than two mean-free-paths, and in two- and three-dimensional geometries, negative fluxes can occur for any mesh size. To correct this problem with DD, set-to-zero, step, and weighted diamond "fixups" have been applied when negative fluxes are observed. These are *ad hoc* remedies which adversely affect accuracy and interact poorly with linear acceleration techniques.

Even the more recently developed numerical schemes such as Linear Discontinuous[2] (LD), Lumped Linear Discontinuous[3] (LLD), Linear[4] and Bilinear[5] Nodal (LN and BN), and Linear Moments[6] (LM) methods are not strictly positive even though all except LLD are third order accurate or better for small meshes. These methods do not require "fixup" because any negative angular flux values are spatially damped and do not propagate as they can in the DD method. As a result, these modern schemes interact well with linear diffusion synthetic acceleration (DSA) techniques.

In this paper a new nonlinear scheme is outlined which is fourth order accurate for small meshes and is strictly positive. The scheme has been implemented, for the one dimensional slab geometry, into the ONELD code and tested on a variety of problems. The method is not limited to one dimensional geometries and work continues on multi-dimensional implementation.

The remainder of this paper will proceed as follows: in Sec.(II) we derive our new nonlinear S_n method, in Sec.(III) we give numerical results to demonstrate the accuracy and positivity of our new scheme, and in Sec.(IV) we give some conclusions and discuss our plans for future work.

II. THE NEW NONLINEAR METHOD

Using standard notation, the slab geometry S_n equations are given by

$$\mu_m \frac{d}{dx}\psi_m(x) + \sigma_t(x)\psi_m(x) = S_m(x) \ , \qquad (1)$$

with appropriate boundary conditions. Here $S_m(x)$ is the neutron source in direction m and can include scattering, an inhomogeneous source, or fission.

To spatially discretize Eq.(1) we use the spatial mesh given in Figure 1. Here we have divided the slab into J cells, each having width $\Delta x_j = x_{j+1/2} - x_{j-1/2}$ and center $x_j = \left(x_{j+1/2} + x_{j-1/2}\right)/2$. Within each cell we require the material properties to be constant, allowing interior material boundaries, if any, to exist only on the cell edges. That is, in the j-th cell we define the total macroscopic cross section $\sigma_t(x) = \sigma_{t,j}$.

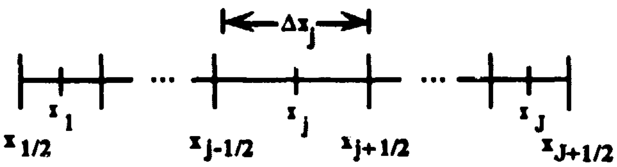

Figure 1. Slab Geometry Spatial Mesh

We will now consider the j-th cell over the interval $x_{j-1/2}$ to $x_{j+1/2}$. The solution within the j-th cell to Eq.(1) for $\mu_m > 0$ is:

$$\psi_m(x) = \psi_m(x_{j-1/2})e^{-\sigma_{t,j}x/\mu_m} + \frac{1}{\mu_m}\int_{x_{j-1/2}}^{x} e^{-\sigma_{t,j}(x_{j+1/2}-x')/\mu_m} S_m(x')dx' \ . \qquad (2)$$

Clearly the solution of the average flux, the outflow at $x_{j+1/2}$, or any angular flux within the cell is strictly positive if $S_m(x)$ is strictly positive. We will now construct a representation of $S_m(x)$ that preserves the first two spatial moments of $S_m(x)$ and is strictly positive.

In the one-dimensional LM method the source in the j-th cell is expanded in Legendre moments as

$$S_m(x) = S_{m,j}\left[P_0(x) + \frac{S^x_{m,j}}{S_{m,j}}P_1(x)\right] \ . \qquad (3)$$

where, $P_0(x) = 1$ and $P_1(x) = 2(x - x_j)/\Delta x_j$ are the zeroth and first order Legendre polynomials, $S_{m,j}$ is the average source and $S^x_{m,j}$ is the source slope. The representation for $S_m(x)$ can be negative if $\left|S^x_{m,j}\right| > S_{m,j}$. To develop a representation that is strictly positive, we first define a normalized source distribution $s_m(x)$ so that $S_m(x) = s_m(x)\, S_{m,j}$. This is given by:

$$s_m(x) = \left[s_0 + s_1 P_1(x)\right] \ . \qquad (4)$$

Here $s_0 = 1$ and $s_1 = S^x_{m,j}/S_{m,j}$ are the zeroth and first Legendre moments of the source.

We will now construct a strictly positive distribution, $\bar{s}_m(x)$, that has the same Legendre moments as the original distribution $s_m(x)$. The information theory[7] prescription for choosing such a distribution is to choose one that maximizes the entropy within the j-th cell, $H_m(x)$, given only the incomplete information that the first two moments provide. Here $H_m(x)$ is given by

$$H_m(x) = \frac{1}{\Delta x_j}\int_{x_{j-1/2}}^{x_{j+1/2}} \bar{s}_m(x)\ln[\bar{s}_m(x)]dx \ , \qquad (5)$$

and

$$\bar{s}_m(x) = \left[\bar{s}_0 + \bar{s}_1 P_1(x)\right] \ . \qquad (6)$$

The two moment constraints are:

$$\Theta^k_m(x) = s_k - \frac{2k+1}{\Delta x_j}\int_{x_{j-1/2}}^{x_{j+1/2}} \bar{s}_m(x)P_k(x)dx = 0 \ . \quad k = 0,1 \qquad (7)$$

We use the Lagrange multipliers, $\lambda_{k,j}$, at the extremum given by

$$\frac{d}{dx}H_m(x)+\sum_{k=0}^{1}\frac{\lambda_{k,j}}{2k+1}\frac{d}{dx}\Theta_m^k(x)=0 \quad . \qquad (8)$$

Next, substituting Eq.(6) into Eq.(5) and Eq.(7) and taking the variation and substituting the result into Eq.(8), we find

$$\tilde{s}(x)=e^{\lambda_{0,j}-1}e^{\lambda_{1,j}P_1(x)} \quad . \qquad (9)$$

The Lagrange multipliers are determined by substituting Eq.(9) into the two moments constraints given by Eq.(7). These are:

$$1=e^{\lambda_{0,j}-1}\left(\frac{\sinh(\lambda_{1,j})}{\lambda_{1,j}}\right) , \qquad (10)$$

and

$$\frac{S_{m,j}^x}{S_{m,j}}=\frac{s_1}{s_0}=3\left[\coth(\lambda_{1,j})-\frac{1}{\lambda_{1,j}}\right] \qquad (11)$$

We can eliminate $\lambda_{0,j}$ in Eq.(9) using Eq.(10) to obtain:

$$\tilde{s}(x)=\frac{\lambda_{1,j}}{\sinh(\lambda_{1,j})}e^{\lambda_{1,j}P_1(x)} \quad . \qquad (12)$$

Substituting $S_m(x)=\tilde{s}_m(x)S_{m,j}$ into Eq.(2) and integrating over the j-th cell, we obtain for $\mu_m>0$

$$\psi_{m,j+1/2}=\psi_{m,j-1/2}e^{-\varepsilon_{m,j}} + \left(\frac{\Delta x_j S_{m,j}}{\mu_m}\right)\left(\frac{\lambda_{1,j}e^{\lambda_{1,j}}}{\sinh(\lambda_{1,j})}\right)\frac{\left[1-e^{-(2\lambda_{1,j}+\varepsilon_{m,j})}\right]}{2\lambda_{1,j}+\varepsilon_{m,j}} \quad . \qquad (13)$$

Here we have defined $\psi(x_{j+1/2})=\psi_{j+1/2}$ and $\varepsilon_{m,j}=\sigma_{t,j}\Delta x_j/\mu_m$.

Similar steps are taken to find the representation for the discrete angular fluxes when $\mu_m<0$.

III. NUMERICAL RESULTS

In this section we provide numerical results for two test problems. For each problem, we compare the new non-linear (NL) method with the linear moments (LM), linear-discontinuous (LD), and diamond difference (DD) with set-to-zero negative flux fixup. The LM and LD schemes do not have fixup routines for negative fluxes and the non-linear scheme is positive-definite. The DD calculations were performed using the ONEDANT code and the NL, LM and LD calculations were performed using the ONELD code. The ONELD code is a variant of ONEDANT that is used for charged particle and neutron transport. ONELD uses the LD scheme in place of the DD scheme used in ONEDANT.

The first test problem is an infinite slab iron-water shield problem and is shown in Figure 2. We use the S_{16} Gauss Legendre quadrature set, three group cross-sections and P_1 scattering. All calculations were converged to a relative error of 10^{-4}.

The results for the first test problem are given in Table 1. Here we give, for each differencing scheme, the neutron leakage from the right side of the slab. The 90 cm water region is 295 mean-free-paths thick in the third neutron group. For coarsest mesh refinement each mesh in this region is 74 mean-free-paths in width. The LN method is seen to be accurate and strictly positive for all mesh refinements. Both the LM and LD methods are accurate and positive for all but the coarsest meshes. The DD method performs poorest of all the methods examined and does not even converge at the coarsest mesh. Note that the NL solution monotonically converges from above as the mesh size is reduced.

The second test problem, which is even more difficult than the first, is shown in Figure 3. This problem has 11 material zones of various widths. We use the S_{16} quadrature set, the BUCLE-80 47 neutron and 20 gamma-ray group cross sections[8] with P_3

scattering. All calculations were converged to a relative error of 10^{-4}.

The results for the second test problem are given in Tables 2 and 3. In Table 2 we give, for each differencing scheme, the neutron leakage from the right side of the slab. In Table 3 we give, for each differencing scheme, the gamma-ray leakage from the right side of the slab. We see that the new NL method is very accurate and positive even for extremely coarse meshing. This is remarkable since the integrated neutron flux in this test problem drops by some twenty four orders of magnitude from the reflective boundary to the vacuum boundary! Both the LM and the LD methods are much better behaved and more accurate than the DD method with LM being more accurate than LD at every mesh. With the exception of the NL method, none of these methods are strictly positive for coarse meshing.

IV. CONCLUSIONS AND PLANS FOR FUTURE WORK

The results of the previous section demonstrate that the new NL method is strictly positive and in the limit of small mesh behaves like the LM method which is fourth order. The real power of the method however, will be in its application to two-, and three- dimensional problems. In multidimensional problems memory and time limitations restrict the degree of mesh refinement obtainable. This is not the case in simple one - dimensional problems.

We plan to use the method of characteristics to solve the transport equation in two- and three-dimensions. In two- and three- dimensions not only the source representation, but also the angular flux representations on the cell faces must be strictly positive. The method of Section II can be used to construct a strictly positive source from the average source and the source moments in two- and three-dimensions. The same technique can be used to construct angular flux representations on the faces using averages values and moments of the angular flux. We are currently working on this extension.

We have recently determined that this new NL method has the diffusion limit; and hence, can be applied to optically thick, highly scattering problems. The ONELD code which was modified to incorporate the NL scheme uses an S_2 iteration accelerator which was constructed for use with the LD method not the NL method. We are developing a more efficient and consistent diffusion acceleration scheme for use with the NL method.

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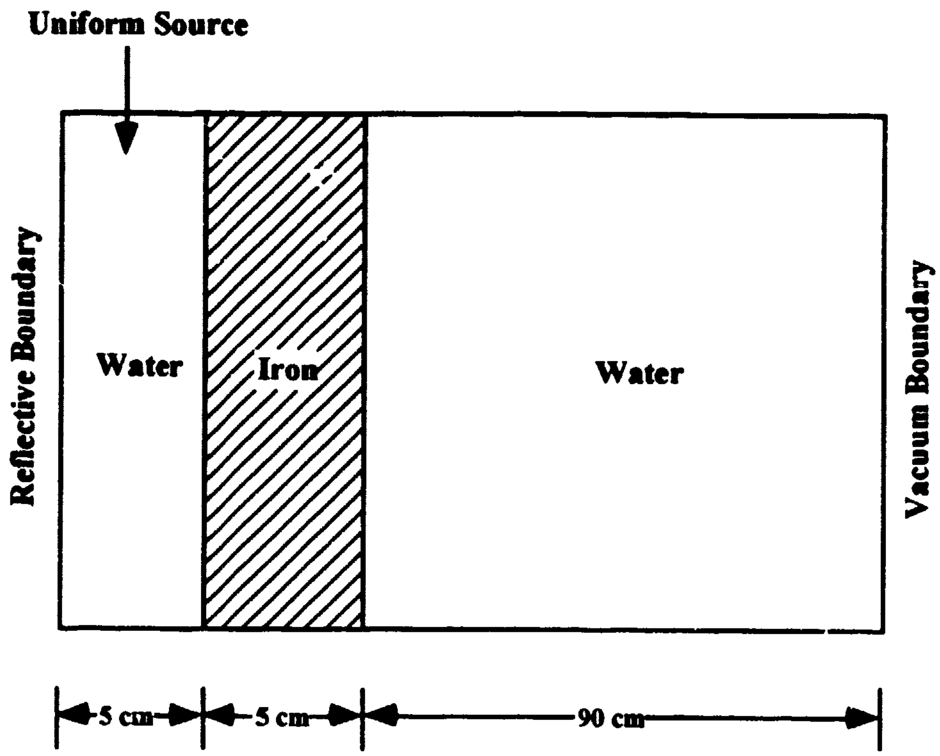

Figure 2. Geometry for Test Problem One.

Table 1: Neutron Leakages (s^{-1}) for Test Problem One

Number of Cells	New NL Method	LM Method	ONELD	ONEDANT
1 + 1 + 4	6.177-7	-1.167-4	-6.191-4	[a]NC
2 + 2 + 8	5.052-7	2.991-7	5.484-8	5.776-11
4 + 4 + 16	4.297-7	3.909-7	3.431-7	2.994-6
4 + 8 + 32	4.055-7	3.972-7	3.900-7	4.291-7
4 + 8 + 64	3.992-7	3.978-7	3.968-7	3.714-7
8 + 16 + 128	3.979-7	3.977-7	3.976-7	3.910-7
8 + 16 + 256	3.977-7	3.977-7	3.977-7	3.961-7

[a]Could not converge problem

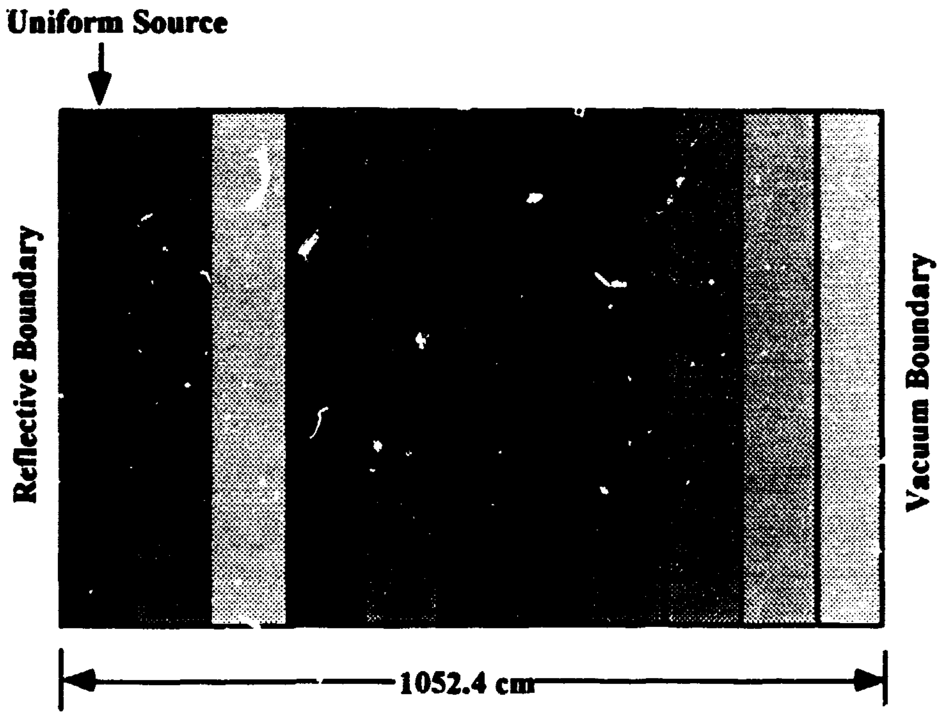

Figure 3. Geometry for Test Problem Two.

Table 2: Neutron Leakages (s^{-1}) for Test Problem Two

Number of Cells	New NL Method	LM Method	ONELD	ONEDANT
34	1.780	4.375	-501.9	2.090×10^4
51	2.571	-1.016	2.090	6.308
100	2.440	2.201	1.308	0.0375
198	2.396	2.372	2.172	0.9090
394	2.390	2.388	2.358	1.881
788	2.390	2.390	2.386	2.252
1576	2.390	2.390	2.389	2.355

Table 3: Gamma-Ray Leakages ($10^2\ s^{-1}$) for Test Problem Two

Number of Cells	New NL Method	LM Method	ONELD	ONEDANT
34	5.569	-4.482	-1.450×10^4	5.175×10^3
51	5.543	2.503	-14.04	2.747
100	5.486	5.196	3.484	0.2900
198	5.413	5.336	5.057	2.533
394	5.339	5.335	5.294	4.421
788	5.325	5.324	5.319	5.080
1576	5.322	5.322	5.321	5.260