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A POSITIVE NON-LINEAR CLOSURE FOR THE S_N EQUATIONS WITH LINEAR-DISCONTINOUS SPATIAL DIFFERENCING

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ABSTRACT

We have developed a new parametric non-linear closure for the 1-D slab-geometry S_n equations with linear-discontinuous (LD) spatial differencing that is strictly positive and yields the set-to-zero fixup equations in the limit as the parameter is increased without bound. Unlike the standard LD equations with set-to-zero fixup, these non-linear S_n equations, for any finite value of the parameter, are differentiable and thus amenable to solution via Newton's method. Furthermore, unlike any exponential-based closure method, our new scheme is robust with respect to negativities in the scattering source that often arise with highly anisotropic scattering. We present results indicating that for an appropriate range of parameteric values, our new method is strictly positive, efficient, and yields solutions that rapidly approach the standard LD solution as the spatial mesh is refined.

Key Words: discrete-ordinates, finite-element, non-linear closures.

1.. INTRODUCTION

The purpose of this paper is to describe a new parametric non-linear closure for the 1-D slab-geometry S_n equations with linear-discontinuous (LD) spatial differencing. Negative fluxes represent a long-standing problem in the numerical transport community. Various fixup procedures have been defined to deal with negativities. One of the oldest is to simply set negative angular flux values to zero whenever they are obtained during the source iteration process. This is called the set-to-zero fixup [1]. This procedure works well in purely absorptive problems, but in problems with scattering, the source iteration process (particularly when accelerated) can interact with the fixup process in such a manner that convergence is never obtained. The linear S_n equations become non-linear when a fixup process is imposed, but the resulting equations are actually non-differentiable and thus not amenable to solution via Newton's method.

There are two strictly positive and differentiable S_n methods based upon the solution of the zero'th and first spatial moment equations: the linear-exponential characteristic method [2] and the exponential linear-discontinuous finite-element method [3]. The characteristic method is very accurate, but expensive in multidimensions, difficult to apply on non-orthogonal meshes, and is not applicable in curvilinear coordinates. The exponential finite-element method is simpler and more widely applicable than the characteristic method, but is less accurate than the characteristic method in certain types of problems. Perhaps most importantly, both of these schemes can fail when small negativities are present in the scattering source due to highly anisotropic scattering expansions.[2].

We have developed a new parametric non-linear closure for the 1-D slab-geometry S_n equations that is strictly positive and yields the set-to-zero fixup equations in the limit as the parameter is increased without bound. Unlike the standard LD equations with set-to-zero fixup, these non-linear S$_n$ equations, for any finite value of the parameter, are differentiable and thus amenable to solution via Newton's method. Furthermore, unlike any exponential-based closure method, our new scheme is robust with respect to negativities in the scattering source that often arise with highly anisotropic scattering. We present results indicating that for an appropriate range of parameteric values, our new method is strictly positive, reasonably efficient, and yields solutions that rapidly approach the standard LD solution in the limit as the spatial mesh is refined.

2. THE NEW CLOSURE

The exact zero'th and first-moment equations in slab-geometry for spatial cell i can be expressed as follows:

$$\mu\left(\psi_{i+1/2} - \psi_{i,i-1/2}\right) + \sigma_{t,i}\psi_{i,a}h_i = Q_{i,a}h_i \ , \tag{1}$$

and

$$3\mu\left(\psi_{i+1/2} - 2\psi_{i,a} + \psi_{i-1/2}\right) + \sigma_{t,i}\psi_{i,x}h_i = Q_{i,x}h_i \ , \tag{2}$$

where $\psi_{i+1/2}$ and $\psi_{i-1/2}$ are the cell edge fluxes, $\psi_{i,a}$ is the flux average, $\psi_{i,x}$ is the flux slope, $Q_{i,a}$ is the total source average, and $Q_{i,x}$ is the total source slope. The inflow cell-edge flux is known from boundary conditions, so these two equations have three unknowns and thus require another to close the system. The standard LD method has the following closure for $\mu > 0$:

$$\psi_{i+1/2} = \psi_{i,a} + \psi_{i,x} \ . \tag{3}$$

This closure yields a negative outflow flux solution whenever $\psi_{i,x}/\psi_{i,a} < -1$. The LD set-to-zero fixup closure for $\mu > 0$ can be expressed as follows:

$$\begin{aligned} \psi_{i+1/2} &= \psi_{i,a} + \psi_{i,x} \ , \quad \text{if } \psi_{i,a} + \psi_{i,x} \geq 0 \ , \\ &= 0 \ , \quad \text{otherwise.} \end{aligned} \tag{4}$$

Our new closure can be expressed as follows for $\mu > 0$:

$$\begin{aligned} \psi_{i+1/2} &= \psi_{i,a} + \psi_{i,x} \ , \quad \text{if} \quad \psi_{i,x}/\psi_{i,a} \geq 0 \ , \\ &= \psi_{i,a}/\left[1 - \psi_{i,x}/\psi_{i,a} + \left(\psi_{i,x}/\psi_{i,a}\right)^2 + \ldots (-1)^N \left(\psi_{i,x}/\psi_{i,a}\right)^N\right] \ , \quad \text{otherwise,} \end{aligned} \tag{5}$$

where N is a parameter. There are four important properties of this closure. The first is that this closure yields an outflow flux of the same sign as the average flux. If the inflow flux is positive and the total source is positive, this will ensure a positive outflow flux. The standard LD closure can yield an outflow flux of sign opposite to that of the average flux. The second property is that the outflow flux is a smooth function of $\psi_{i,a}$ and $\psi_{i,x}$. The degree of smoothness depends upon N. More specifically, the closure has N continuous derivatives at the transition point, $\psi_{i,x}/\psi_{i,a} = 0$. Thus, unlike traditional set-to-zero fixup techniques, this closure yields non-linear moment equations that can be solved via Newton's method. The third property is that in the limit as $N \to \infty$, this closure converges to the set-to-zero closure defined in Eq. (4). Finally, the fourth property is that given an inflow flux of one sign, and an average flux of another sign (the sign change presumably due to non-physical negativities in the cross section expansion) the scheme will yield an outflow flux that carries the sign of the average flux. Exponential-based closures can yield singular equations under these conditions. The quantity $\psi_{i+1/2}/\psi_{i,a}$ is plotted versus $\psi_{i,x}/\psi_{i,a}$ in Fig. 1 for the LD closure, the set-to-zero closure, the $N = 2$ $(N2)$, $N = 4$ $(N4)$ and $N = 10$ $(N10)$ closures. The smoothness of the new closure and its approach to the set-to-zero closure with increasing N is clear. Due to space limitations, we only give closure relationships for $\mu > 0$, but one can easily construct the equations for $\mu < 0$ by analogy.

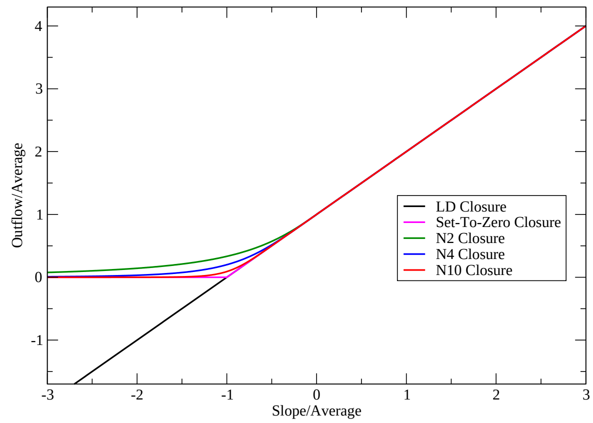

Figure 1. Closure relationsips.

3. COMPUTATIONAL RESULTS

We present results for two problems. The first corresponds to a total slab thickness of $12.0\ cm$, $\sigma_t = 1.0\ cm^{-1}$, $\sigma_s = 0.0\ cm^{-1}$, with an isotropic flux incident from the left and Gauss S_8 quadrature. Several calculations with various closures were performed for this problem with the number of cells varying as follows: $N_{cells} = 2, 4, 8, 16, 32, 64$. The scalar fluxes for the LD method, the linear exponential discontinuous (ED) method, the $N4$ method and the $N10$ method are plotted in Fig. 2. The linear representation within each cell for the angular fluxes in each direction (used to compute the scalar fluxes) were obtained for all closures by interpolating the outflow and average fluxes. The negativity of the LD solution and the positivity of the new closure solutions is evident. The

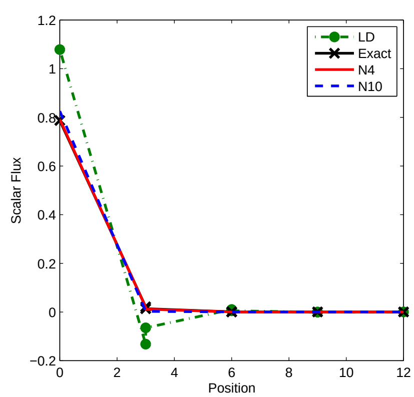

Figure 2. Flux solutions for problem 1.

second problem we consider is identical to the first except that $\sigma_s = 0.5\ cm^{-1}$. An analytic solution is available for this problem [4]. The L_2 errors for the cell-averaged scalar fluxes as a function of the number of cells are plotted in Fig. 3 for the LD method, the ED method, the $N4$ method and the $N10$ method. Note that the $N4$ and $N10$ solutions converge to the LD solution as the mesh is refined. As expected the $N10$ solution converges to the LD solution more

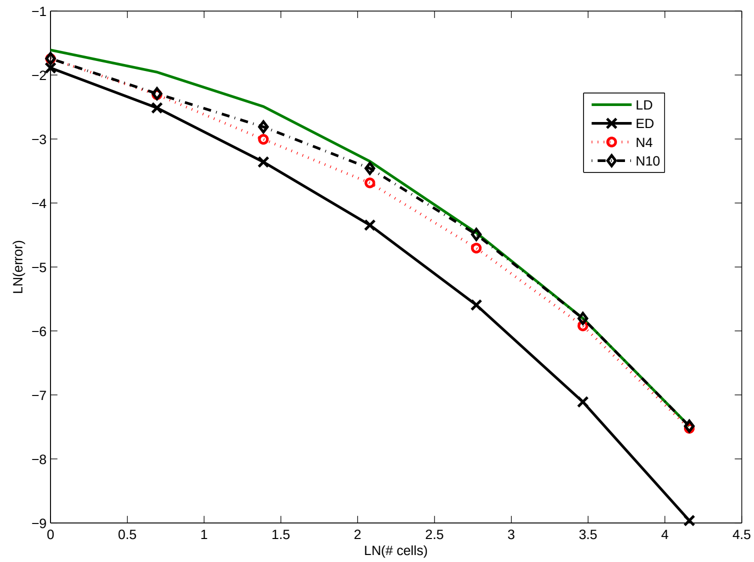

Figure 3. Error versus cell width for various closures.

rapidly than the $N4$ solution. The ED solution is also the most accurate of all solutions in this case, but this is a problem-dependent result, as demonstrated by additional calculations not shown here. The S$_n$ equations for all methods are solved by source iteration. The sweep equations consist of a 2×2 system for each spatial cell and quadrature direction. In the non-linear case, these 2×2 systems are solved by Newton iteration. Each Newton iteration requires the solution of a linear 2×2 system. We have recorded the total number of linear 2×2 solutions performed for each method in each calculation that was performed. Relative to the LD method, the ED method requires from 5 to 11 more 2×2 solves, the $N4$ method requires from 1.8 to 1.9 more 2×2 solves, and the $N10$ method requires very nearly 1.5 times more 2×2 solves. Thus the new method is significantly more economical than the ED method. One might suppose that the minimum number of Newton iterations that can be taken is two, and therefore that no non-linear method should perform less than less than twice the number of 2×2 solutions performed with the LD method. However, an advantage of our new closure is that if the slope after the first linear solution for a given cell and direction during a sweep has a particular sign, no further iteration is required. In contrast, the ED method requires at least two iterations under all circumstances. Although we do not present the results here, we have performed calculations with highly anisotropic scattering that demonstrate the ability of the new closure to tolerate negativities in the scattering sources.

4. CONCLUSIONS

Our new non-linear LD closure is very promising. It largely preserves the LD solution when a fixup is not needed, it is much less costly than the ED method, it is not much more costly than the LD method, and it tolerates the scattering source negativities that can arise with highly anisotropic scattering and render exponential-based methods singular. The optimal choice for N will clearly be problem-dependent, and we intend to investigate this question in the future.

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