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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 such values 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 generally less accurate than the characteristic method. 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:

$$\psi_{i+1/2} = \psi_{i,a} + \psi_{i,x} \quad \text{for } \mu > 0, \tag{3a}$$

and

$$\psi_{i-1/2} = \psi_{i,a} - \psi_{i,x} \quad \text{for } \mu < 0. \tag{3b}$$

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

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

and as follows for $\mu < 0$:

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

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

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

and as follows for $\mu < 0$

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

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 $N \rightarrow \infty$, this closure converges to the set-to-zero closure defined in Eqs. (4a) and (4b). 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 $\psi_{i,x}/\psi_{i,a}$ for $\mu > 0$ 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.

3. COMPUTATIONAL RESULTS

We present results for three 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 at the left boundary a vacuum condition at the right, and a Gauss S_8 quadrature. Several calculations with various closures were performed for this problem using uniform spatial meshes (equal cell widths) with the number of cells varying as follows: $N_{cells} = 2, 4, 8, 16, 32, 64$. The scalar fluxes for the LD method, the

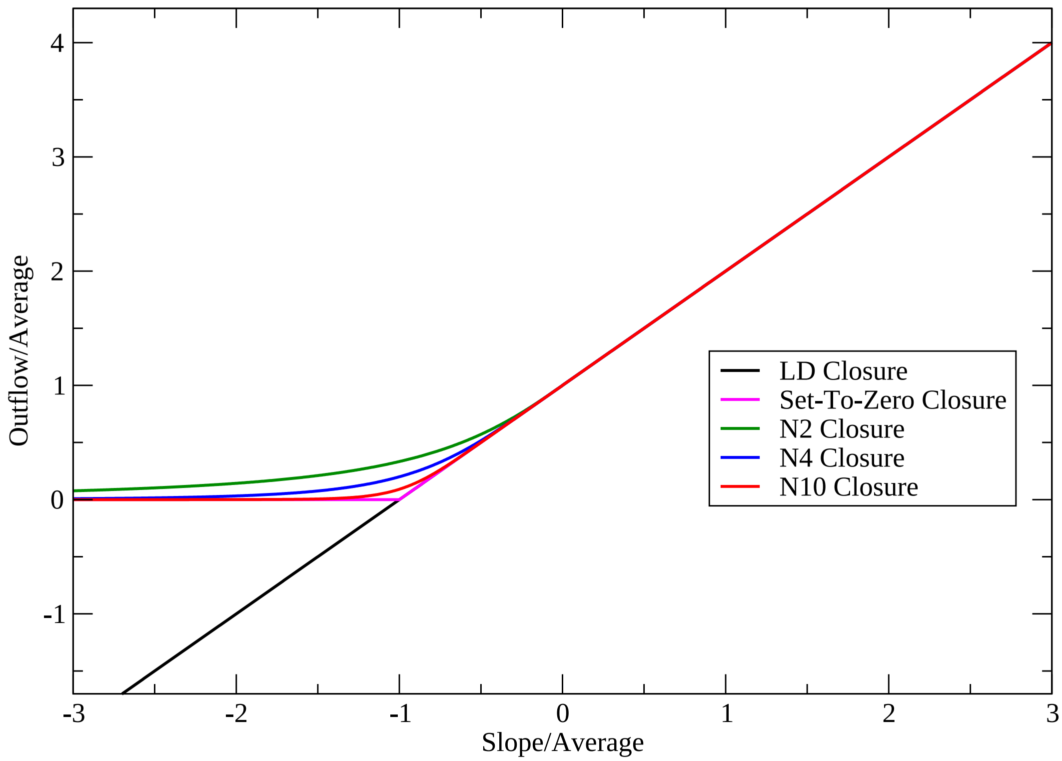

Figure 1. Closure relationsips.

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 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. These errors, which we denote by ϵ_{L_2}, are computed as follows:

$$\epsilon_{L_2} = \sqrt{\sum_{i=1}^{N_{cells}} \left(\phi_i^{ex} - \phi_i^{cp}\right)^2 \Delta x_i} \ , \tag{6}$$

where ϕ_i^{ex} is the exact cell-averaged flux for cell i, ϕ_i^{cp} is the computational cell-averaged flux for cell i, and Δx_i is the width for cell i. Note from Fig. 3 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 rapidly than the $N4$ solution. The ED solution is also the most accurate of all

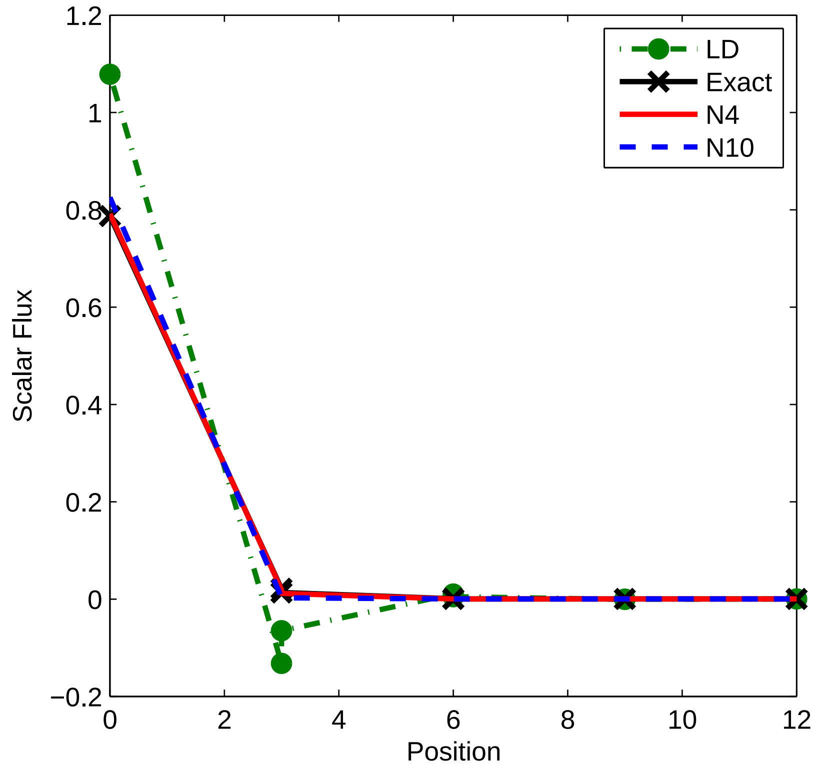

Figure 2. Flux solutions for problem 1.

solutions in this case, but this is a problem-dependent result as demonstrated by our third problem. This problem is identical to problem 1 except that there is a vacuum condition at both boundaries, a constant isotropic distributed source, and $\sigma_s = 0.9\ cm^{-1}$. The L_2 errors for the cell-averaged scalar fluxes as a function of the number of cells are plotted in Fig. 4 for the LD method, the ED method, the $N4$ method and the $N10$ method. It can be seen from Fig. 4 that the ED method is the least accurate of all the methods. The ED solution always has spatial curvature, whereas the LD solution has no spatial curvature at all. Thus the ED method can be signficantly more accurate than the LD method when the curvature of the ED solution matches that of the analytic solution (see problem 2) and significantly less accurate when the curvature of the ED solution does not match that of the analytic solution (see problem 3).

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

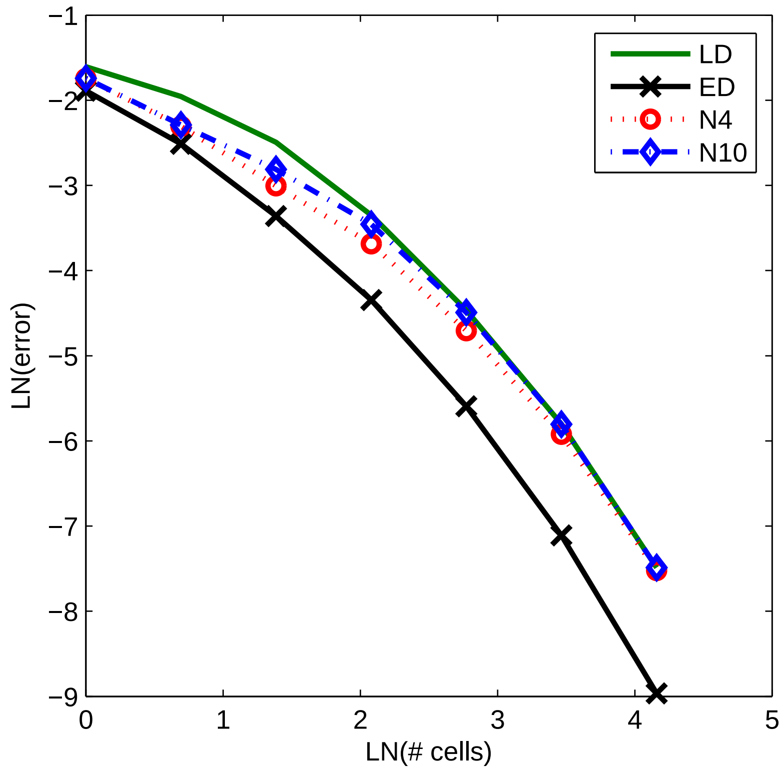

Figure 3. Error versus number of cells for problem 2

2×2 system. We have recorded the total number of linear 2×2 solutions performed with each method for problem 2. The results are given in Table I. It can be see from Table I that, relative to the LD method, the ED method requires from 11.4 to 11.7 more 2×2 solves, the $N4$ method requires from 1.9 to 2.8 more 2×2 solves, and the $N10$ method requires from 1.5 to 2.5 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

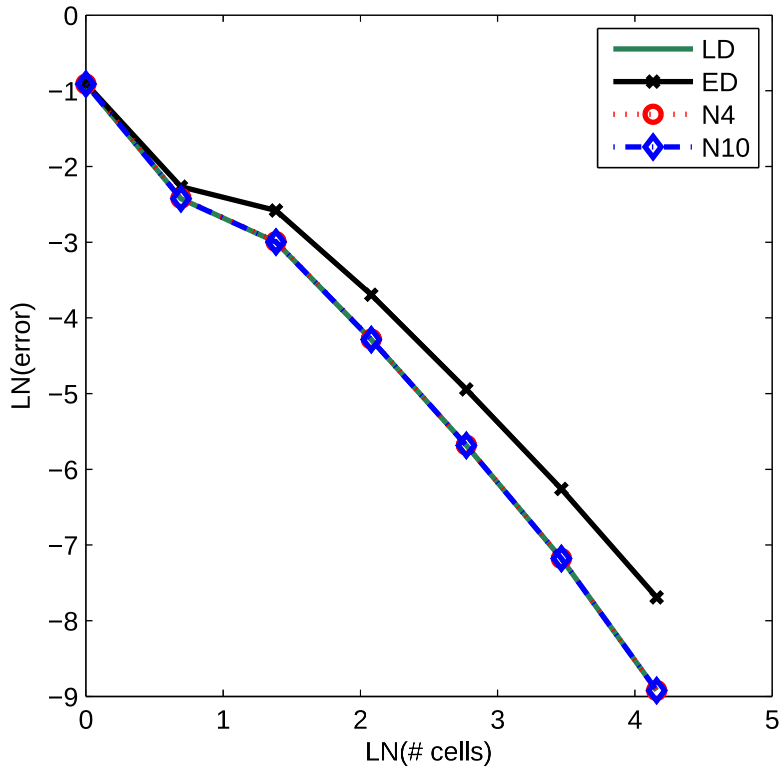

Figure 4. Error versus number of cells for problem 3.

Table I. Total number of 2×2 matrix inversions for problem 2.

No. Cells	LD	ED	N2	N4	N10	N20
1	152	1785	456	437	380	342
2	320	4651	1188	1194	753	589
4	800	9627	2679	2673	2627	2111
8	1728	21445	5302	5361	4833	3923
16	3456	39978	9626	9137	6853	5310
32	6912	78998	16078	15065	10533	10415
64	13824	156981	27595	26172	20809	20736

scattering sources. This is a property of high practical importance. We suspect that strictly positive exponential-based discretizations have never achieved widespread use within the nuclear engineering community largely because they can fail even with very small negativities in the scattering source.

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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