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TITLE: A DIFFUSION ACCELERATED SOLUTION METHOD FOR THE NONLINEAR CHARACTERISTIC SCHEME

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A Diffusion Accelerated Solution Method for the Nonlinear Characteristic Scheme

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ABSTRACT

Recently the nonlinear characteristic scheme for spatially discretizing the discrete-ordinate equations was introduced. This scheme is accurate for both optically thin and optically thick spatial meshes and produces strictly positive angular and scalar fluxes. The nonlinear characteristic discrete-ordinate equations can be solved using the source iteration method; however, it is well known that the this method converges prohibitively slowly for optically thick problems with scattering ratios at or near unity. In this paper we describe a diffusion accelerated solution method for solving the nonlinear characteristic equations in slab geometry.

I. INTRODUCTION

Recently a nonlinear spatial differencing scheme for solving the discrete-ordinate equations was introduced[1,2]. This scheme, referred to as the nonlinear characteristic (NC) scheme, is accurate for both optically thin and optically thick spatial meshes. The NC scheme is based upon the analytic solution to the discrete-ordinate equations and preserves the zeroth and first spatial moments of the angular flux. The source within each cell is approximated by an exponential representation, derived from information theory[3]. The NC scheme is exact for problems with a truly exponential source and for purely absorbing problems. It also possesses the thick diffusion limit; thus, it will be very accurate for problems with optically thick, highly scattering meshes. The NC scheme possesses many highly desirable qualities. To make it even more desirable, an efficient method to solve the NC equations must be developed, especially for optically thick, high scattering problems.

Originally, the NC scheme was solved using source iteration (SI); however, it is well known that the SI method converges prohibitively slowly for optically thick problems with scattering ratios at or near unity. Later the NC scheme was solved using the SI method accelerated with a linear S_2 linear discontinuous (LD) accelerator. This worked for many problems but was not always stable or efficient. Many linear DSA accelerators were tried, but all failed due to instabilities. Also, nonlinear accelerators were tried with varying degrees of success; one such method has been reported[4] and is the basis for the solution method we describe in this paper.

The NC equations are nonlinear in terms of a parameter we call λ, which depends nonlinearly on S^x / S, the ratio of the first source moment and the zeroth source moment. The basic idea of our solution method is as follows: we linearize the NC equation about a fixed λ. The linearized system is then solved using a linear DSA method. After solving the linearized system, a new λ is obtained and a new linearized system is solved with this new fixed λ. This process is continued until λ, and ultimately, the scalar fluxes, are converged.

The remainder of this paper is as follows: in Sec. II we provide the equations for the NC scheme, in Sec. III we describe the new diffusion accelerated solution method for solving the NC equations, in Sec. IV we provide numerical results, and in Sec. V we draw some conclusions based on these results.

II. THE NONLINEAR CHARACTERISTIC SCHEME

The NC scheme is based upon the analytic solution to the discrete-ordinate equations. The source within each cell is approximated by an exponential representation, is derived from information theory, and preserves the zeroth and first spatial moments of the angular flux. This source is given by:

$$S(x) = \frac{\lambda}{\sinh(\lambda)} e^{\lambda P_1(x)} \ , \tag{1}$$

where $P_1(x)=(2x/\Delta x)-1$ and λ will be defined later. The monoenergetic NC discrete-ordinate equations for the i-th spatial cell with isotropic scattering and a spatially constant source take the following form:

$$\frac{\mu_m}{\Delta x_i}\left(\psi_{m,i+1/2} - \psi_{m,i-1/2}\right) + \sigma_{t,i}\psi_{m,i} = S_i \ , \tag{2}$$

$$\frac{3\mu_m}{\Delta x_i}\left(\psi_{m,i+1/2} + \psi_{m,i-1/2} - 2\psi_{m,i}\right) + \sigma_{t,i}\psi^x_{m,i} = S^x_i \ , \tag{3}$$

$$\psi_{m,i\pm 1/2} = \psi_{m,i\mp 1/2} e^{-|\varepsilon_{m,i}|} + S_i \Delta x_i \xi_{m,i}(\pm\lambda_i) \ , \ \mu_m \gtrless 0 \ , \tag{4}$$

$$S_i = \frac{\sigma_{s,i}\phi_i}{2} + \frac{Q_i}{2} \ , \tag{5}$$

$$S^x_i = \frac{\sigma_{s,i}\phi_{x,i}}{2} \ , \tag{6}$$

$$\frac{S^x_i}{S_i} = 3\left[\coth(\lambda_i) - 1/\lambda_i\right] \equiv \beta(\lambda_i) \ , \tag{7}$$

$$\phi_i = \sum_{m=1}^{N} \psi_{m,i} w_m \ , \tag{8}$$

and

$$\phi^x_i = \sum_{m=1}^{N} \psi^x_{m,i} w_m \ . \tag{9}$$

Here, for the i-th cell, $\psi_{m,i\pm 1/2}$, $\psi_{m,i}$, and $\psi^x_{m,i}$ are the edge angular fluxes, the average angular flux, and the first angular flux moment respectively; ϕ_i and ϕ^x_i are the average scalar flux and first scalar flux moment, S_i and S^x_i are the average source and first source moment and Q_i is the fixed source. We have defined $\varepsilon_{m,i} = (\sigma_{t,i}\Delta x_i)/\mu_m$. The nonlinear function $\xi_{m,i}(\lambda_i)$ is given by the following equation:

$$\xi_{m,i}(\lambda_i) = \frac{1}{|\mu_m|}\frac{\lambda_i}{\sinh(\lambda_i)} e^{\lambda_i}\left[\frac{1-e^{-(\lambda_i+|\varepsilon_{m,i}|)}}{\lambda_i+|\varepsilon_{m,i}|}\right] . \tag{10}$$

III. NONLINEAR CHARACTERISTIC SOLUTION METHOD

The first step in deriving our solution method is to linearize the NC equations about some fixed $\lambda=\lambda^{(k)}$, where k is the iteration number. This is done by using the Newton-Raphson method to expand Eqs.(7) and (10) into the following linear equations:

$$\frac{S_i^x}{S_i} \approx \beta(\lambda_i^{(k)}) + \Delta\lambda_i^{(k+1)}\,\beta'(\lambda_i^{(k)}) \ . \tag{11}$$

$$\xi_{m,i}(\lambda_i) \approx \xi_{m,i}(\lambda_i^{(k)}) + \Delta\lambda_i^{(k+1)}\xi'_{m,i}(\lambda_i^{(k)}) \ , \tag{12}$$

where,

$$\beta'(\lambda_i^{(k)}) = \left(\frac{d\beta(\lambda_i)}{d\lambda_i}\right)^{(k)} \ , \tag{13}$$

$$\xi'_{m,i}(\lambda_i^{(k)}) = \left(\frac{d\xi_{m,i}(\lambda_i)}{d\lambda_i}\right)^{(k)} \ , \tag{14}$$

$$\Delta\lambda_i^{(k+1)} = (\lambda_i^{(k+1)} - \lambda_i^k) \ . \tag{15}$$

Solving Eq.(15) for $\Delta\lambda_i^{(k+1)}$, we obtain

$$\Delta\lambda_i^{(k+1)} = \frac{\left[S_i^x / S_i - \beta(\lambda_i^{(k)})\right]}{\beta'(\lambda_i^{(k)})} \ , \tag{16}$$

Eq.(10) now becomes

$$\xi_{m,i}(\lambda_i) \approx \xi_{m,i}(\lambda_i^{(k)}) + \frac{\left[S_i^x / S_i - \beta(\lambda_i^{(k)})\right]}{\beta'(\lambda_i^{(k)})}\xi'_{m,i}(\lambda_i^k) \ . \tag{17}$$

With the above approximations, we now define an iteration process for λ_j. The equations for iteration (k+1) are given by:

$$\frac{\mu_m}{\Delta x_i}\left(\psi_{m,i+1/2}^{(k+1)} - \psi_{m,i-1/2}^{(k+1)}\right) + \sigma_{t,i}\psi_{m,i}^{(k+1)} = S_i^{(k+1)} \ , \tag{18}$$

$$\frac{3\mu_m}{\Delta x_i}\left(\psi_{m,i+1/2}^{(k+1)} + \psi_{m,i-1/2}^{(k+1)} - 2\psi_{m,i}^{(k+1)}\right) + \sigma_{t,i}\psi_{m,i}^{x,(k+1)} = S_i^{x,(k+1)} \ , \tag{19}$$

$$\psi_{m,i\pm1/2}^{(k+1)} = \psi_{m,i\mp1/2}^{(k+1)}e^{-|\varepsilon_{m,i}|} + S_i^{(k+1)}\Delta x_i\left[\xi_{m,i}(\lambda_i^{(k)}) + \frac{\left[S_i^{x,(k+1)} / S_i^{(k+1)} - \beta(\lambda_j^{(k)})\right]}{\beta'(\lambda_i^{(k)})}\xi'_{m,i}(\lambda_i^k)\right] \ , \ \mu_m \gtrless 0 \ , \tag{20}$$

$$\Delta\lambda_i^{(k+1)} = \frac{\left[S_i^{x,(k+1)} / S_i^{(k+1)} - \beta(\lambda_i^{(k)})\right]}{\beta'(\lambda_i^{(k)})} \ , \tag{21}$$

$$\lambda_i^{(k+1)} = \lambda_i^{(k)} + \Delta\lambda_i^{(k+1)}, \tag{22}$$

We note that Eqs.(18)-(20) need to be solved at each (k+1) iteration. These equations are linear; therefore, we can use a linear DSA method to efficiently solve them. It has recently been shown that in x-y geometry, the bilinear nodal (BLN) equations can be solved by a DSA method designed for solving the bilinear discontinuous (BLD) equations[5]. This has also been shown to be true for the bilinear characteristic (BLC) equations[6]. We note that the BLD, BLN and BLC methods all preserve the same spatial moments. Thus, our first attempts for the DSA equations were the Adams and Martin[7] method, used for solving the linear discontinuous (LD) equations, and the Khalil[8] method, used for solving the linear moments (LM) equations, since both of these methods preserve the same spatial moments as Eqs.(18)-(20). Both of these methods are unstable for large λ. To obtain DSA equations that are consistent with Eqs.(18)-(20) and lead to a stable method for large λ, we follow the approach Khalil used for obtaining DSA equations for the LM equations. More specifically, we use Eq.(1) for the representation of the source instead of the linear representation used by Khalil. This leads to a nonlinear diffusion equation, which we linearize in the same manner as the NC equations. The linearized equations are then used to accelerate Eqs.(18)-(20). We note that when λ is zero, the linearized NC equations are equivalent to the LM equations

A summary of our solution method is as follows:

Step 1: Start with an initial guess of $\lambda_j^{(k)} = \lambda_j^{(0)} = 0$.

Step 2: Solve Eqs.(18)-(20) using linear DSA accelerated transport iterations (DSA transport iterations), converging the scalar fluxes to within a relative error of ε. Retain the scalar fluxes for a starting guess for the next k iteration.

Step 3: Calculate $\Delta\lambda_j^{(k+1)}$ using Eq.(21).

Step 4: Calculate new estimate for $\lambda_j^{(k+1)}$ using Eq.(22).

Step 5: Repeat Steps 2 to 4 until $\max_j(\Delta\lambda_j^{(k+1)} / \lambda_j^{(k+1)} \leq \varepsilon)$. Steps 2 to 4 comprise one k-iteration.

We note that when $\lambda_j^{(k)} = 0$, Eqs.(18)-(20) are algebraically equivalent to the LM equations and the linearized DSA equations are identical to Khalil's DSA equations for the LM scheme. Therefore, for many problems, the initial guess of $\lambda_j^{(k)} = 0$ will be a very good approximation and the iteration on λ will converge very rapidly. We also note that Eq.(7) is a transcendental equation that cannot be directly inverted to obtain a single expression for λ. To solve the NC equations by the SI method, some polynomial fit must be used to invert this equation. For our solution method, we do not need to directly invert Eq.(7) and therefore we obtain the exact (to within iteration error) solution to this transcendental equation. In the next section we provide results that demonstrate the efficiency of our new method.

IV. NUMERICAL RESULTS

In this section we provide solutions to three different test problems to show the effectiveness and efficiency of our solution method. The solution to the first problem will show that our solution method works very well for homogeneous problems with a scattering ratio equal to unity. This is where SI fails miserably. The solution to the second problem shows that our method works well for heterogeneous problems, that is, problems with difference regions of differing cross sections and sources. The third problem shows how our method works for deep penetration problems. It is important that the method perform well for deep penetration problems since this is where the accuracy of the NC is greater than that of other existing methods, especially for optically thick meshes. For deep penetration problems with optically thick meshes the NC method becomes strongly nonlinear, and this is where previously attempted methods have failed to be stable or effective.

The first test problem is a 100 cm thick homogeneous slab with vacuum boundaries, a total cross section of 1 cm^{-1}, a scattering ratio of 1 and a uniform source of 1.0 cm^{-3}. We solve this problem with both the S_4 and S_{16} Gauss-Legendre quadrature sets. Table 1 and Table 2 give the number of k-iterations and total number of DSA accelerated transport iterations to solve the problem at various mesh widths. The convergence criterion for all iterations is 10^{-4}. We cannot solve this problem with SI in less than 10,000 iterations. We see from Table 1 that our method is very effective at reducing the number of transport iterations from that of SI. It appears that our method is stable for

Table 1: Iterations to Converge Problem One

	S_4 Quadrature		S_{16} Quadrature	
Δx (mfp)	number of k-iterations to converge λ.	total number of DSA linear transport iterations	number of k-iterations to converge λ.	total number of DSA linear transport iterations
0.1	4	6	5	6
0.5	5	6	5	6
1.0	5	6	5	6
2.0	5	6	5	6
5.0	5	6	6	7
10.0	5	7	6	8
20.0	6	8	6	8
50.0	6	8	6	8

The second test problem is a 100 cm slab with vacuum boundaries that consists of three regions. The first region, 0<x<25cm, has a total cross section of 1 cm^{-1}, a scattering ratio of 0.8 and a uniform source of 0.1 cm^{-3}; the second region, 25<x<40 cm, has a total cross section of 1 cm^{-1}, a scattering ratio of 0.99 and a uniform source of 1.0 cm^{-3}; and the third region, 40 <x<100 cm, has a total cross section of 1 cm-1, a scattering ratio of 0.70 and a uniform source of 0.01 cm^{-3}. We solve this problem with the S_{16} Gauss-Legendre quadrature set. Table 3 gives the number of k-iterations and number of DSA accelerated linearized NC transport iterations to converge the problem for various meshes. The convergence criterion for all iterations is 10^{-4}. We ran the problem with SI and at the 16+16+32 mesh, SI took 499 transport iterations and 141 cpu seconds on a CRAY YMP computer. For the same mesh, the new method took 8 DSA accelerated linear transport iterations and 3.70 cpu seconds. Again Table 3 shows that our solution method is very effective at reducing the number of iterations compared to the SI method. Our method is very efficient for this problem as well.

Table 3: Iterations to Converge Test Problem Two

number of mesh cells reg 1+reg 2+reg 3	maximum cell width (mfp)	number of k-iterations to converge λ	number of DSA linear transport iterations
1+1+2	30.0	6	8
2+2+4	15.0	8	10
4+4+8	7.5	9	12
8+8+16	3.75	7	10
16+16+32	1.875	5	7
32+32+64	0.9375	5	7

The third test problem is a 60 cm slab with a total cross section of 1 cm-1 and a scattering ratio of 0.95. There is an incident istotropic flux on the left boundary of 1 cm^{-2} s^{-1}. and a vacuum boundary on the right. There are no internal sources. We solve this problem with the S_{16} Gauss-Legendre quadrature set. Table 4 gives the number of k-iterations and number of DSA accelerated linearized NC transport sweeps to converge the problem as well as the total leakage from the problem for various meshes. All calculations are converged to a relative error of 10^{-4}. We provide the leakage from the problem to show how accurate the NC scheme in terms of spatial discretization error. We see from Table 4 that the solution method performs quite well for this problem. For this problem, the scalar flux drops off some 10 orders of magnitude from the origin to the right side of the slab. We see that for only two mesh cells at 30 mfps per cell, the total leakage given by the NC scheme is off by less than 40 percent. Again, we ran this problem with SI and found that for the spatial mesh with 64 cells, SI took 443 iterations and 124.4 cpu seconds. That for our new method took 20 DSA linear transport iterations and 6.23 cpu seconds.

Table 4: Iterations to Converge Test Problem Three

number of mesh cells	mesh width (mfp)	number of k-iterations	number of DSA linear transport iterations	total leakage from the slab (x10-11s^{-1})
2	50.0	8	19	5.68
4	25.0	6	17	5.56
8	12.5	5	17	4.67
16	6.25	5	17	4.20
32	3.125	7	18	4.09
64	1.5625	7	20	4.07
128	0.78125	6	20	4.07

V. CONCLUSIONS AND FUTURE WORK

In this paper we have described a new solution method for solving the NC discrete-ordinates equations in slab geometry. This method is diffusion accelerated and is very effective at reducing the total number of transport iterations from that of the SI method when the scattering ratio is at or near unity. Our method is also very efficient, since we can directly invert the DSA equations at a reasonable cost in slab geometry. We have shown that this method works for heterogeneous as well as homogeneous problems. We have also showed that this method works well for deep penetration problems with optically thick spatial meshes. This last feature is very important since previously tried methods all failed or performed poorly for deep penetration problems.

The NC scheme has been extended to x-y geometry[9]. In future work, we plan to extend our solution method to solve the x-y geometry NC discrete-ordinate equations. In x-y geometry the solution method for the DSA (diffusion) equations becomes much more important in the overall efficiency of the method since we cannot afford to directly invert these equations.

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