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TITLE: AN ANALYSIS OF THE FINITE-DIFFERENCED, EVEN-PARITY DISCRETE-ORDINATES EQUATIONS IN SLAB GEOMETRY

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An Analysis of the Finite-Differenced, Even-Parity, Discrete-Ordinates Equations in Slab Geometry

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Considerable effort has been expended in recent years in finding improved spatial differencing schemes for the neutron and radiation transport equations. Standard criteria used to select a candidate scheme are its order of spatial convergence for small mesh size and its positivity in the sense that positive solutions emerge from positive input data.[1] More recently, it has become clear that truly robust schemes must behave well in diffusing regions (e.g. have the correct diffusion limits) and must be compatible with an effective iteration acceleration method (e.g., diffusion synthetic acceleration [DSA]).[2,3] Recently, Morel and Larsen reported their work on a promising new method called the multiple balance method that has virtually all the desirable characteristics. The one drawback they report is a lack of general positivity.[4]

Here we study a different approach to the problem by considering discrete-ordinates approximations to the even-parity transport equations. We analyze three spatial difference approaches: diamond differencing, cell-edge differencing, and cell-center differencing. For the case of isotropic scattering and sources, the latter two approaches are shown to be strictly positive, to be second-order accurate, to be compatible with derived diffusion synthetic acceleration methods, and to possess the necessary diffusion limits. Unlike previous work with the even-parity equation, we do not use finite elements or variational principles.[1]

Considering slab geometry with isotropic sources and scattering, the even-parity discrete-ordinates equations are

$$-\mu_m^2 \frac{d}{dx}\left(\frac{1}{\sigma}\frac{d\chi_m}{dx}\right) + \sigma(x)\,\chi_m(x) = \sigma_s(x)\,\phi(x) + Q(x) = S(x) \qquad (1)$$

$$m = 1, 2, \ldots, M/2$$

where χ_m is the even-parity flux and is even in angle and the scalar flux is given by

$$\phi(x) = \tfrac{1}{2}\int_{-1}^{1} d\mu\,\psi(x,\mu) = \int_0^1 d\mu\,\chi(x,\mu) \approx \sum_{m=1}^{M/2} w_m \chi_m(x) \qquad (2)$$

The derivation of Eq. (1), presented elsewhere,[1] involves straightforward algebra performed on the first-order transport equation for positive and negative directions.

If one discretizes the first-order transport equation using diamond-differencing, the even-parity diamond-difference equations can be derived using a procedure analogous to that used in deriving the analytic equations:

$$\frac{-\mu_m^2}{\sigma_i h_i}(\chi_{m,i+1/2} - \chi_{m,i-1/2}) + \frac{\mu_m^2}{\sigma_{i-1} h_{i-1}}(\chi_{m,i-1/2} - \chi_{m,i-3/2}) + \frac{\sigma_i h_i}{4}(\chi_{m,i+1/2} + \chi_{m,i-1/2}) + \frac{\sigma_{i-1} h_{i-1}}{4}(\chi_{m,i-1/2} + \chi_{m,i-3/2}) =$$

$$\frac{h_i}{4}(S_{i+1/2} + S_{i-1/2}) + \frac{h_{i-1}}{4}(S_{i-1/2} + S_{i-3/2})$$

$$m = 1, 2, \ldots, M/2$$
$$i = 2, \ldots, I \qquad (3)$$

It is important to note that Eq. (3) is algebraically equivalent to the first-order form of the diamond-difference equations.

A second approach to differencing Eq. (1) is to use cell-edge differencing, analogous to what one would use with the diffusion equation. This results in a modification of the removal term:

$$-\frac{\mu_m^2}{\sigma_i h_i}(\chi_{m,i+1/2} - \chi_{m,i-1/2}) + \frac{\mu_m^2}{\sigma_{i-1} h_{i-1}}(\chi_{m,i-1/2} - \chi_{m,i-3/2}) + \tfrac{1}{2}(\sigma_i h_i + \sigma_{i-1} h_{i-1})\, \chi_{m,i-1/2} = \tfrac{1}{2}(h_i + h_{i-1})\, S_{i-1/2} \qquad (4)$$

$m = 1, 2, \ldots, M/2$

$i = 2, 3, 4, \ldots, I$

A third approach is to use cell-center differencing resulting in

$$-2\mu_m^2 \left\{ \frac{(\chi_{m,i+1} - \chi_{mi})}{(\sigma_i h_i + \sigma_{i+1} h_{i+1})} - \frac{(\chi_{mi} - \chi_{m,i-1})}{(\sigma_i h_i + \sigma_{i-1} h_{i-1})} \right\} + \sigma_i h_i \chi_{mi} = h_i S_i \qquad (5)$$

$m = 1, 2, \ldots, M/2$

$i = 2, \ldots, I-1$

Clearly, appropriate differenced boundary equations must be used with Eqs. (3), (4), and (5).

Considering positivity, it is straightforward to show that the damond-difference approximation does not guarantee a positive solution.[1] However, because both Eqs. (4) and (5) form so-called S matrices, they must give positive solutions. Further, because their derivation is completely analogous to familiar derivations of cell-edge and cell-center diffusion equation differencing, it is clear that the differencing is second-order accurate.[5]

Both Eqs. (4) and (5) have been analyzed in the thick and intermediate diffusion limits, and both possess the required diffusion limits. The analyses of the boundary layers for both cases seem to indicate that the cell-edge differencing approach behaves better than cell-center differencing when diffusing boundary layers are unresolved.

The DSA equations for Eqs. (4) and (5) are derived by simply angularly integrating them. This results in:

$$-1.0/(3.0\,\sigma_i h_i)\,(\phi_{0,i+1/2}^{\ell+1} - \phi_{0,i-1/2}^{\ell+1}) + 1.0/(3.0\,\sigma_{i-1} h_{i-1})\,(\phi_{0,i-1/2}^{\ell+1} - \phi_{0,i-3/2}^{\ell+1}) + \tfrac{1}{2}(\sigma_{ai} h_i + \sigma_{a,i-1} h_{i-1})\,\phi_{0,i-1/2}^{\ell+1} =$$

$$\tfrac{1}{2}(h_i Q_i + h_{i+1} Q_{i-1}) + 2.0/(3.0\,\sigma_i h_i)\,(\phi_{2,i+1/2}^{\ell+1} - \phi_{2,i-1/2}^{\ell+1}) - 2.0/(3.0\,\sigma_{i-1} h_{i-1})\,(\phi_{2,i-1/2}^{\ell+1} - \phi_{2,i-3/2}^{\ell+1}) \qquad (6)$$

$i = 2, \ldots, I$

and

$$-2.0/(3.0)\left\{\frac{(\phi_{oi+1}^{\ell+1}-\phi_{oi-1}^{\ell+1})}{(\sigma_j h_i+\sigma_{i+1}h_{i+1})}-\frac{(\phi_{oi}^{\ell+1}-\phi_{oi-1}^{\ell+1})}{(\sigma_i h_i+\sigma_{i-1}h_{i-1})}\right\}+\sigma_{ai}h_i\phi_{oi}^{\ell+1}=h_iQ_i+\frac{4.0}{3.0}\left\{\frac{(\phi_{2i+1}^{\ell+1}-\phi_{2i}^{\ell+1})}{(\sigma_i h_i+\sigma_{i+1}h_{i+1})}-\frac{(\phi_{2i}^{\ell+1}-\phi_{2i-1}^{\ell+1})}{(\sigma_i h_i+\sigma_{i-1}h_{i-1})}\right\} \quad (7)$$

The symbols used in Eqs. (6) and (7) are standard.[3] Fourier analyses of these iteration schemes indicate that the acceleration methods are as effective as DSA with diamond differencing.

A simple problem previously solved to compare DSA approaches was used to compare the three methods.[3] The problem is an 8-cm slab, with a vacuum boundary on the left and reflective boundary on the right. Eight equal mesh cells are used, with varying total cross sections and a secondary ratio 0.98. A distributed source is present in the right four cells. The Table depicts the number of iterations for 0.0001 pointwise convergence using DSA with the three schemes and S_4 quadrature. As previously reported,[3] unaccelerated, the problems require hundreds of iterations.

It is clear that finite-differenced even-parity discrete-ordinates is a strong candidate for future use in production computer codes.

TABLE

NUMBER OF DIFFUSION SYNTHETIC ACCELERATION ITERATIONS

FOR TEST PROBLEM

σ_t\Method	Diamond Differencing	Cell-Edge Differencing	Cell-Center Differencing
1.0	4	4	3
4.0	6	3	3
6.0	6	3	2
20.0	5	2	2

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