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Quadratic Finite Element Method for 1D Deterministic Transport

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INTRODUCTION

In the discrete ordinates, or S_N , numerical solution of the transport equation, both the spatial (r) and angular (Ω) dependence on the angular flux $\psi(r, \Omega)$ are modeled discretely. While significant effort has been devoted toward improving the spatial discretization of the angular flux [1, 2], we focus on improving the angular discretization of $\psi(r, \Omega)$. Specifically, we employ a Petrov-Galerkin quadratic finite element approximation for the differencing of the angular variable (μ) in developing the one-dimensional (1D) spherical geometry S_N equations. We develop an algorithm that shows faster convergence with angular resolution than conventional S_N algorithms.

SPHERICAL TRANSPORT EQUATION

This 1D spherical transport equation in conservative form is given by

$$\frac{\mu}{r^2} \frac{\partial}{\partial r} [r^2 \psi(r, \mu)] + \frac{1}{r} \frac{\partial}{\partial \mu} [(1 - \mu^2) \psi(r, \mu)] + \Sigma(r) \psi(r, \mu) = S(r, \mu). \quad (1)$$

We discretize the angular variable with an $N+1$ set of directions or quadrature such that

$$\mu_1 < \mu_2 < \dots < \mu_n < \dots < \mu_N; \mu_{1/2} = -1, \text{ and}$$

$$\mu_{N+1} = 1. \quad \mu_{1/2} = -1 \text{ is the starting direction and is}$$

treated separately from the other directions. [3, 4] The angular flux for the direction μ_n is $\psi(r, \mu_n) = \psi_n$. (The spatial dependence is omitted.)

Conventional Methods

The standard formulation of the S_N equations involves the diamond-difference (DD) relationship between the angular fluxes for angle n and “half-angles” $n - 1/2$ and $n + 1/2$:

$$\psi_{n+1/2} = 2\psi_n - \psi_{n-1/2}. \quad (2)$$

To preserve the solution of a uniform isotropic flux in an infinite medium ($\psi(r, \mu) = S/\Sigma$) for any quadrature set, differencing coefficients $\alpha_{n+1/2}$ are used in the angular derivative term to force the two streaming terms to vanish. [3, 4] Upon spatial differencing, we obtain the conventional S_N equations. In addition, Moreland and Monty have developed a “weighted diamond-difference” algorithm that is more accurate than standard DD. [5]

DESCRIPTION OF THE ACTUAL WORK

Our new method employs Petrov-Galerkin finite elements for $\psi(r, \mu)$ in Eq. (1). Specifically, we approximate the angular dependence as a combination of a continuous piecewise bilinear function and a continuous quadratic function of μ :

$$\psi(r, \mu) \cong \psi_n \left(\frac{\mu_{n+1} - \mu}{\Delta\mu_n} \right) + \psi_{n+1} \left(\frac{\mu - \mu_n}{\Delta\mu_n} \right) + \tilde{\psi}_n \left[\frac{4(\mu_{n+1} - \mu)(\mu - \mu_n)}{\Delta\mu_n^2} \right], \quad (3)$$

where $\mu_n \leq \mu \leq \mu_{n+1}$ and $\Delta\mu_n = \mu_{n+1} - \mu_n$. To obtain the S_N equations, Eq. (3) is substituted for $\psi(r, \mu)$ in Eq. (1), and then we operate on Eq. (1) by

$$\int_{\mu_n}^{\mu_{n+1}} (\cdot) d\mu \text{ for all } \mu \neq -1. \text{ The result is the following:}$$

$$\frac{\Delta\mu_n}{6r^2} \frac{d}{dr} \{ r^2 [\psi_n A(\mu) + \psi_{n+1} B(\mu) + 2\tilde{\psi}_n C(\mu)] \} + \frac{1}{r} [\psi_{n+1} (1 - \mu_{n+1}^2) - \psi_n (1 - \mu_n^2)] + \frac{\Sigma(r) \Delta\mu_n}{2} [\psi_n + \psi_{n+1} + \frac{4}{3} \tilde{\psi}_n] = S(r) \Delta\mu_n, \quad (4)$$

where $A(\mu) = \mu_{n+1} + 2\mu_n$, $B(\mu) = 2\mu_{n+1} + \mu_n$, and $C(\mu) = \mu_{n+1} + \mu_n$. This equation has one known angular flux (ψ_n) and two unknown angular fluxes (ψ_{n+1} and $\tilde{\psi}_n$). Thus, we need another equation. That equation is obtained by substituting Eq.(3) for $\psi(r, \mu)$ in Eq.(1), and then operating on Eq.(1) by $\int_{\mu_n}^{\mu_{n+1}} (\cdot) \mu d\mu$.

The result is

$$\begin{aligned} & \frac{\Delta\mu_n}{12r^2} \frac{d}{dr} \{r^2[\psi_n D(\mu) + \psi_{n+1} E(\mu) + \frac{4}{5} \tilde{\psi}_n F(\mu)]\} + \\ & \frac{1}{r} \{ \psi_{n+1} [\mu_{n+1}(1 - \mu_{n+1}^2) - \frac{\Delta\mu_n}{2} + \frac{\Delta\mu_n}{12} E(\mu)] - \psi_n \\ & [\mu_n(1 - \mu_n^2) + \frac{\Delta\mu_n}{2} - \frac{\Delta\mu_n}{12} D(\mu)] - \tilde{\psi}_n [\frac{2\Delta\mu_n}{3} - \\ & \frac{\Delta\mu_n}{15} F(\mu)] \} + \frac{\Sigma(r)\Delta\mu_n}{6} [\psi_n A(\mu) + \psi_{n+1} B(\mu) \\ & + 2\tilde{\psi}_n C(\mu)] = \frac{S(r)(\mu_{n+1}^2 - \mu_n^2)}{2}, \end{aligned} \quad (5)$$

where $D(\mu) = \mu_{n+1}^2 + 2\mu_{n+1}\mu_n + 3\mu_n^2$,
 $E(\mu) = 3\mu_{n+1}^2 + 2\mu_{n+1}\mu_n + \mu_n^2$, and
 $F(\mu) = 3\mu_{n+1}^2 + 4\mu_{n+1}\mu_n + 3\mu_n^2$.

Upon spatial differencing Eqs.(4) and (5), we have the S_N equations for our quadratic finite element method. These equations are solved similarly to the conventional S_N equations by marching through the grid in the direction of particle motion. However, in this new method, two unknowns exist (ψ_{n+1} and $\tilde{\psi}_n$); thus, we must solve a system of equations given by Eqs.(4) and (5) for each radial zone.

RESULTS

To test this method, let us consider a simple test problem proposed by Lathrop.[4] The problem, called "Test3", is a two-region spherewith the following features.

Table 1: Test Problem Specifications

	Radii	Source	Cross Section
Region1	0<r<1	10	1
Region2	1<r<2	0	5

The media in both regions are pure absorbers, so this problem neglects scattering.

For several different quadrature sets, we determine the absorption and leakage rates for both the weighted DD and our new quadratic finite element (QFE) schemes. The results are represented in Table 2. We include Lathrop's results from his quadratic continuous (QC) algorithm.[4]

Table 2: Absorption and Leakage Rates for Test Problem

Number of Angles	Diamond Difference	Quad. Finite Element	Quad. Continuous
Absorption Rate			
2	41.8858	41.8199	41.752
4	41.8485	41.8103	41.8032
8	41.8248	41.8102	41.8096
16	41.8153	41.8101	41.8099
32	41.8123	41.8101	
Exact	41.8101	41.8101	41.8101
Leakage Rate			
2	0.00710	0.06803	0.13576
4	0.03935	0.07757	0.08451
8	0.06305	0.07773	0.07806
16	0.07356	0.07775	0.07777
32	0.07645	0.07776	
Exact	0.07776	0.07776	0.07776

These results indicate the QFE scheme converges much faster than the weighted DD scheme with finer angular resolution. For example, the leakage rate from the QFE scheme is within 0.3% of the exact solution when using four angles. However, the leakage rate from the weighted DD scheme is an enormous 49% below the analytical solution when using four angles. Even for 32 angles, the leakage rate from weighted DD remains 1.7% below the exact solution. For QFE, the leakage rate is highly converged with just eight angles. Also, it appears that our quadratic finite element scheme converges faster than Lathrop's QC method. For four angles, the leakage rate from QC is about 8.7% too high. Further study and comparison should be made to understand the discrepancies between our algorithm and Lathrop's algorithm. One idea is that we obtain our two equations by taking the zeroth- and first-order angular moments of Eq. (1). Lathrop obtains his two equations by taking the zeroth-order angular moments of both Eq. (1) and the first angular derivative of Eq.(1). Lathrop, however, thinks these different equations lead to small numerical differences.[4] Other differences may involve the spatial differencing of four S_N equations and the choice of quadrature sets.

In summary, we have developed a new higher-order S_N algorithm for the solution of the 1D spherical transport equation using quadratic finite elements. This method shows excellent convergence with relatively coarse angular resolution. This convergence rate has been shown to be superior to conventional S_N techniques for 1D spherical geometry. In the future, we plan to test these ideas in problems containing scattering and in criticality problems.

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