A Modified Step Characteristic Method for Solving the S_N Transport Equation

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INTRODUCTION

The step characteristic (SC) method is a wellestablished robust (positivity preserving) spatial discretization scheme to solve the S_N transport equation [1]. The convergence properties, in terms of accuracy and efficiency, of the SC method have been intensively studied in many literatures before [2-4].

In general, SC is a 2nd order accurate scheme, and more accurate than the diamond difference (DD) method in weak and medium scattering problems. However, SC becomes less accurate for diffusive problems (the scattering ratio tends to 1). Although it is well known that SC does not have the thick diffusion limit, a recent study by Wang shows that SC possesses the intermediate diffusion limit [6]. To improve the accuracy of SC for thick diffusive problems, Wang proposed a modification to the weighting factor of SC, which makes SC to attain the thick diffusion limit [6].

In this paper, we carry out a detailed numerical study to demonstrate the accuracy of the modified SC scheme, which is called "mSC" herein.

MODIFIED SC SCHEME (mSC)

The monoenergetic S_N equation in slab geometry with the assumption of isotropic scattering and constant external neutron source is written as

$$\mu_n \frac{d\psi_n}{dx} + \Sigma_t \psi_n = \frac{\Sigma_s}{2} \sum_{n'=1}^N \psi_{n'} w_{n'} + \frac{Q}{2}, \qquad (1)$$

where

 μ_n = neutron direction cosine with respect to *x*;

 ψ_n = angular flux;

 $w_{n\prime}$ = quadrature weights;

 Σ_{t} = total macroscopic cross section;

 Σ_{s} = macroscopic scattering cross section;

Q =constant external neutron source.

The SC discretization of the S_N equation on the onedimensional mesh (see Fig. 1) is given as follows.

$$j-1 \qquad j \qquad j+1$$

$$\bullet \qquad \qquad \bullet$$

$$j-1/2 \qquad j+1/2$$

Fig. 1. One-dimensional mesh.

$$\frac{\mu_n}{h_j} \left(\psi_{n,j+1/2} - \psi_{n,j-1/2} \right) + \sum_{t,j} \left[\left(\frac{1 - \alpha_{n,j}}{2} \right) \psi_{n,j-1/2} + \left(\frac{1 + \alpha_{n,j}}{2} \right) \psi_{n,j+1/2} \right] = \frac{\sum_{s,j}}{2} \sum_{n'=1}^{N} \left[\left(\frac{1 - \alpha_{n',j}}{2} \right) \psi_{n',j-\frac{1}{2}} + \left(\frac{1 + \alpha_{n',j}}{2} \right) \psi_{n',j+1/2} \right] w_{n'} + \frac{Q_j}{2},$$
(2)

where

$$\alpha_{n,j} = \frac{1 + e^{-\Sigma_{t,j}h_j/\mu_n}}{1 - e^{-\Sigma_{t,j}h_j/\mu_n}} - \frac{2\mu_n}{\Sigma_{t,j}h_j} = \frac{1 + e^{-\tau_j/\mu_n}}{1 - e^{-\tau_j/\mu_n}} - \frac{2\mu_n}{\tau_j}; \quad (3)$$

$$\tau_i = \Sigma_{t,i} h_i$$
, cell optical thickness; (4)

$$h_j = \text{mesh size of cell } j.$$
 (5)

Take the S10 Gauss-Legendre quadrature set as an example. Fig. 2 shows the weighting factor α as a function of the computational cell optical thickness τ . The SC tends to the 1st-order step difference (SD) scheme at $\alpha = \pm 1$. On the other hand, the SC becomes the 2nd-order DD scheme when α limits to zero as $\tau \rightarrow 0$.





Notice that the SC produces the exact solution if the problem becomes a pure absorbing one, i.e., $\Sigma_s = 0$.

Deterministic Transport Methods

To improve the accuracy of SC for thick and diffusive problems, we introduce the scaling term $1 - c^{\beta}$ into the SC weighting factor as proposed in Ref. [6]:

$$\alpha_{n,j} = \frac{1 + e^{-\tau_j \left(1 - c_j^{\beta}\right)/\mu_n}}{1 - e^{-\tau_j \left(1 - c_j^{\beta}\right)/\mu_n}} - \frac{2\mu_n}{\tau_j \left(1 - c_j^{\beta}\right)},\tag{6}$$

where the exponential constant β is a positive number larger than 1; we can take for example $\beta = 3$. $c_j \equiv \frac{\Sigma_{s,j}}{\Sigma_{t,j}}$, which is the scattering ratio in cell *j*.

As $c \rightarrow 1$, the $1 - c^{\beta}$ term tends to zero, and thus $\alpha \rightarrow 0$. As a result, the SC reverts to the DD scheme, and therefore it is expected that it will attain the thick diffusion limit as DD does. If the solution of a thick diffusive problem contains abrupt changes or thin layers at the boundary or in the interior, we can adjust the $1 - c^{\beta}$ term by introducing a smoothness indicator into Eq. (6), as defined for the LF-WENO3 scheme [7]. However, it is not needed for nondiffusive problems since the new scheme will retain the robustness of the original SC method.

NUMERICAL DEMOSTRATION

Our first problem is a simple one-group onedimensional (1-D) fixed source problem to numerically demonstrate the spatial accuracy of the new mSC scheme. The vacuum boundary is used for both sides of the slab. The Gauss–Legendre S₁₂ quadrature set is used for angular discretization, and isotropic scattering is assumed. The size of the domain is 1cm, and it is uniformly divided into 10 mesh cells. The macroscopic cross section, $\Sigma_t = 5 \text{ cm}^{-1}$, and the scattering ratio is varied from 0 to 1. The external source $Q = 1 \text{ cm}^{-1}$. Note that the flux is dimensionless.

For each scattering ratio, we compute the L1 errors of the numerical scalar flux with respect to the exact solutions. Fig. 3 shows the L1 errors for DD, SC, and mSC, respectively.



Fig. 3. Scalar flux L1 error vs. scattering ratio.

It is seen that the errors yielded from SC has a great dependence upon the scattering ratio, while the DD errors stay nearly insensitive to this parameter (slightly decrease when c becomes large). SC is more accurate than DD for the scattering ratio c < 0.7, while it becomes increasingly worse after c becomes larger than 0.7. Our new mSC scheme has significantly improved the accuracy of SC for larger scattering ratios, and overall it is much more accurate than DD and SC.

The second problem is also a 1-D slab problem to demonstrate the property of positivity preserving (robustness). The domain size is 8 cm, and it is divided into 80 uniform cells. As for problem 1, the Gauss–Legendre S_{12} quadrature set is used for angular discretization. In this problem, there is strongly absorbing region in the center and two more diffusive regions on the outside, resulting in the thin boundary and interior layers, as shown in Fig. 4.





As expected, DD produces oscillatory and negative results (blue curve), whereas mSC performs as robustly as the original SC does. Notice that the cell-average flux of DD is less oscillatory than its cell-edge flux because the oscillation is largely cancelled out by arithmetically averaging both edge values of each computational cell. The third problem is to demonstrate that mSC possesses the thick diffusion limit. The problem is also a 1-D slab problem with the vacuum boundary on both sides of the domain. The specifications of the poblem are given as:

$$\begin{split} & L = 1, & h = 0.1, \\ & \Sigma_t = \frac{1}{\varepsilon}, & \Sigma_s = \frac{1}{\varepsilon} - 0.8\varepsilon \\ & Q = \varepsilon, \end{split}$$

where L is the slab thickness and h is the mesh size in dimension of cm. The dimension of Σ_t and Σ_s is cm⁻¹. The problem becomes thick and diffusive as ε decreases.

Two values of ε are considered for comparison. Figs. 5a and 5b show the results for $\varepsilon = 0.01$ and 0.001, respectively. It clearly shows that mSC can attain the thick diffusion limit, but the original SC does not. The reason is that mSC tends to the DD scheme at the diffusion limit.

If solutions contain both thick diffusive and nondiffusive regions, at the interface we can employ a smoothness indicator to adjust the $1 - c^{\beta}$ term to improve the robustness of mSC.



Fig. 5. Diffusion limit.

CONCLUSIONS

In this paper, we have presented a modified step characteristic method, called mSC, to improve the accuracy of the original SC scheme. The idea is that we have introduced a scaling factor, $1 - c^{\beta}$ in the α term of SC, to adjust the cell optical thickness. When the problem becomes more diffusive, namely $c \rightarrow 1$, the scaling factor will prevent the increase of cell optical thickness, and thus the weight factor α won't tend to ± 1 with c, resulting in the SD method that is first order accurate and has no thick diffusion limit. The numerical results have demonstrated that the new mSC scheme can preserve great robustness of the original SC, and is much more accurate than SC and DD as well. More importantly it can attain the thick diffusion limit, which is of significant computational interest for thick diffusive problems such as radiative transfer. The study of its performance for 2-D and 3-D problems will be our future work.

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