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CONVERGENCE OF INNER ITERATIONS SCHEME OF THE DISCRETE ORDINATE METHOD IN SPHERICAL GEOMETRY*1)

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Abstract

In transport theory, the convergence of the inner iteration scheme to the spherical neutron transport equation has been an open problem. In this paper, the inner iteration for a positive step function scheme is considered and its convergence in spherical geometry is proved.

Mathematics subject classification: 65N12, 65N22, 65F10.
Key words: Transport equation, Discrete ordinate, Inner iteration.

1. Introduction

In 1968, Carlson and Lathrop [1, p. 261] pointed out, there were some unsolved problems in neutron transport theory. One of them is the convergence of inner and outer iteration process. Perhaps investigations of these problems lead to procedures for accelerating convergence. Since then considerable progress has been made in convergence of inner iterations in slab geometry. For example, Menon and Sahni [2] estimated the spectral radius of the iteration matrix and proved the convergence theorem under the assumption of "non-regenerative" in slab geometry. Nelson [3] proved that the similar conclusion under the hypothesis of "weak non-multiplying". Recently Yuan et al[4] proved the convergence under a weaker condition on known data and more general boundary conditions.

Due to the appearance of the angular derivative in curvilinear geometry, the formalism of such inner iterations scheme are more complex and there is not any known convergent result by now. In this paper, we will establish the convergence of inner iterations to the spherical neutron transport equation. The means employed here is the Perron-Frobenius theory for non-negative matrix, but the argument method of Nelson's proof [3] is improved, just like that in [4] so as to handle complicated process. Although the result is concluded for a positive step scheme, it can be extended to some other positive schemes.

Consider the following neutron transport equation

$$\mu\frac{\partial\psi}{\partial r}+\frac{1-\mu^2}{r}\frac{\partial\psi}{\partial\mu}+\sigma(r)\psi=\frac{1}{2}c(r)\int_{-1}^{1}\psi(r,\mu')d\mu'+f(r), \tag{1}$$

where $r\in[0,R]$, $\mu\in[-1,1]$, ψ is angular flux with subject to vacuum boundary condition

$$\psi(R,\mu)=0, \quad \mu<0. \tag{2}$$

Here $\sigma(r)\geq c(r)\geq 0$ are the total and the scattering cross section respectively, $f(r)$ is the non-negative external source.

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Eq.(1) is usually expressed the following conservative form too,

$$\frac{\mu}{r^2}\frac{\partial r^2\psi}{\partial r}+\frac{1}{r}\frac{\partial(1-\mu^2)\psi}{\partial\mu}+\sigma(r)\psi=\frac{1}{2}c(r)\int_{-1}^{1}\psi(r,\mu')d\mu'+f(r). \tag{1'}$$

Consider a spatial and angular net with mesh points $0=r_{\frac{1}{2}}<r_{\frac{3}{2}}<\cdots<r_{K+\frac{1}{2}}=R$; $-1=\mu_{\frac{1}{2}}<\mu_{\frac{3}{2}}<\cdots<\mu_{N+\frac{1}{2}}=1$, where N is an even number. Let $C_k=[r_{k-\frac{1}{2}},r_{k+\frac{1}{2}}]$ for $k=1,2,\cdots,K$. Suppose that in the interior of each C_k, $\sigma(r)$ and $c(r)$ are constants σ_k and c_k respectively, then the standard inner iteration schemes are as follows [5, pp. 230 or 9, pp. 141]:

$$\begin{gathered}\mu_m(A_{k+\frac{1}{2}}\psi^{(n+1)}_{k+\frac{1}{2},m}-A_{k-\frac{1}{2}}\psi^{(n+1)}_{k-\frac{1}{2},m})\\ +(A_{k+\frac{1}{2}}-A_{k-\frac{1}{2}})\cdot\frac{\alpha_{m+\frac{1}{2}}\psi^{(n+1)}_{k,m+\frac{1}{2}}-\alpha_{m-\frac{1}{2}}\psi^{(n+1)}_{k,m-\frac{1}{2}}}{\omega_m}\\ +V_k\sigma_k\psi^{(n+1)}_{km}=S^{(n)}_k,\end{gathered} \tag{3}$$

$$S^{(n)}_k=V_kc_k\sum_{j=1}^{N}\psi^{(n)}_{kj}\omega_j+V_kf_k.$$

$$m=1,2,\cdots,N;k=1,2,\cdots,K.$$

where $\mu_m\in[\mu_{m-\frac{1}{2}},\mu_{m+\frac{1}{2}}]$ are even order Gaussian quadrature sets, and ω_m are the corresponding weights, $\sum_{m=1}^{N}\omega_m=1$. $A_{k\pm\frac{1}{2}}=r^2_{k\pm\frac{1}{2}},V_k=\frac{1}{3}(r^3_{k+\frac{1}{2}}-r^3_{k-\frac{1}{2}})$, $\alpha_{m+\frac{1}{2}}-\alpha_{m-\frac{1}{2}}=-\mu_m\omega_m$ and $\alpha_{\frac{1}{2}}=0$.

Boundary conditions are

$$\psi^{(n+1)}_{K+\frac{1}{2},m}=0,\quad m=1,2,\cdots,\frac{N}{2}. \tag{4}$$

The symmetry conditions at the center of the sphere are

$$\psi^{(n+1)}_{\frac{1}{2},N+1-m}=\psi^{(n+1)}_{\frac{1}{2},m},\quad m=1,2,\cdots,\frac{N}{2}. \tag{5}$$

In order to complete the differencing procedure, we need two auxiliary relationships

$$\psi^{(n+1)}_{km}=a\psi^{(n+1)}_{k+\frac{1}{2},m}+(1-a)\psi^{(n+1)}_{k-\frac{1}{2},m}, \tag{6}$$

$$\psi^{(n+1)}_{km}=b\psi^{(n+1)}_{k,m+\frac{1}{2}}+(1-b)\psi^{(n+1)}_{k,m-\frac{1}{2}}. \tag{7}$$

where $0\le a\le 1,0\le b\le 1,k=1,\cdots,K;m=1,\cdots,N$.

The starting direction equation ($\mu=-1$) is given by

$$-(A_{k+\frac{1}{2}}\psi^{(n+1)}_{k+\frac{1}{2},\frac{1}{2}}-A_{k-\frac{1}{2}}\psi^{(n+1)}_{k-\frac{1}{2},\frac{1}{2}})+V_k\sigma_k\psi^{(n+1)}_{k,\frac{1}{2}}=S^{(n)}_k. \tag{8}$$

$$\psi^{(n+1)}_{k,\frac{1}{2}}=a\psi^{(n+1)}_{k+\frac{1}{2},\frac{1}{2}}+(1-a)\psi^{(n+1)}_{k-\frac{1}{2},\frac{1}{2}}, \tag{9}$$

$$k=1,2,\cdots,K.$$

The boundary condition for the starting equation (8) is

$$\psi^{(n+1)}_{K+\frac{1}{2},\frac{1}{2}}=0. \tag{10}$$

It is useful to illustrate solving procedure. On the space-angle mesh beginning with $\psi^{(n+1)}_{K+\frac{1}{2},\frac{1}{2}} = 0$, we march inward (decreasing k) in the $\mu = -1$ starting direction using Eqs. (8) and (9) to obtain $\psi^{(n+1)}_{k-\frac{1}{2},\frac{1}{2}}$ and $\psi^{(n+1)}_{k,\frac{1}{2}}$ for $k = K, K-1, \cdots, 1$. Knowing $\psi^{(n+1)}_{k+\frac{1}{2},m}$ and $\psi^{(n+1)}_{k,m-\frac{1}{2}}$ then we can calculate the $\psi^{(n+1)}_{k-\frac{1}{2},m}$, $\psi^{(n+1)}_{km}$ and $\psi^{(n+1)}_{k,m+\frac{1}{2}}, k = K, K-1, \cdots, 1; m = 1, \cdots, N/2$ by Eqs. (3, 4, 6, 7) until all of the angular fluxes for $\mu_m < 0$ are obtained. Next we calculate the starting fluxes at $k = \frac{1}{2}$ for $m > N/2$ from Eq. (5), then we march outward (increasing k) using Eqs. (3, 4, 6, 7) for $\psi^{(n+1)}_{k+\frac{1}{2},m}$, $\psi^{(n+1)}_{km}$ and $\psi^{(n+1)}_{k,m+\frac{1}{2}}$ $k = 1, \cdots, K; m = N/2+1, \cdots, N$. Replacing the scalar flux $\psi^{(n+1)}_{km}, k = 1, 2, \cdots, K; m = 1, 2, \cdots, N$ to update the scattering source $S^{(n)}_k$ for the next iteration.

Formally, by letting $n \to \infty$ in (3) and (8) we get

$$\begin{gathered}\mu_m(A_{k+\frac{1}{2}}\psi_{k+\frac{1}{2},m} - A_{k-\frac{1}{2}}\psi_{k-\frac{1}{2},m}) \\ +(A_{k+\frac{1}{2}} - A_{k-\frac{1}{2}}) \cdot \frac{\alpha_{m+\frac{1}{2}}\psi_{k,m+\frac{1}{2}} - \alpha_{m-\frac{1}{2}}\psi_{k,m-\frac{1}{2}}}{\omega_m} \\ +V_k\sigma_k\psi_{km} = S_k,\end{gathered} \tag{11}$$

$$-(A_{k+\frac{1}{2}}\psi_{k+\frac{1}{2},\frac{1}{2}} - A_{k-\frac{1}{2}}\psi_{k-\frac{1}{2},\frac{1}{2}}) + V_k\sigma_k\psi_{k,\frac{1}{2}} = S_k. \tag{12}$$

$$S_k = V_k c_k \sum_{j=1}^{N} \psi_{kj}\omega_j + V_k f_k.$$

Remark 1. Eq. (11) is a discrete scheme for Eq. (1') obtained by finite volume method, although $\mu_{k+\frac{1}{2}}, k = 1, \cdots, K-1$ are not given explicitly. Eq. (12) corresponds to (1') in the case of $\mu = -1$. By now we still do not see the strict convergence proof of the scheme (11) to Eq. (1) in literature, but some properties in similar scheme to slab geometrical neutron transport equation [8] have been investigated. We guess the solution of (11) is convergent under some conditions.

Remark 2. Eqs. (6) and (7) describe approximate relations among boundary fluxes $\psi_{k\pm\frac{1}{2},m}$, $\psi_{k,m\pm\frac{1}{2}}$ and scalar flux ψ_{km}. For $a = b = \frac{1}{2}$, schemes (3)-(10) are the so-called diamond difference ones. The diamond method is more accurate than that choosing other parameters a and b, but cannot guarantee positive solutions to (3) and (8). If a, b are chosen

$$a = 1, \qquad b = 1, \quad \mu_m > 0; \tag{13}$$

$$a = 0, \qquad b = 1, \quad \mu_m < 0, \tag{14}$$

the schemes are called step function ones, which are non-negative.

Remark 3. Denote all $\psi_{km}, \psi_{k+\frac{1}{2},m}, \psi_{k,m+\frac{1}{2}}$ as a vector $\mathbf{\Psi}$, then Eqs.(3) and (8) can be expressed briefly as

$$\mathbf{H\Psi^{(n+1)}} = \mathbf{S\Psi^{(n)}} + \mathbf{V}.$$

where

$$\mathbf{\Psi} = \begin{pmatrix} \mathbf{\Psi_1} \\ \mathbf{\Psi_2} \end{pmatrix}, \mathbf{H} = \begin{pmatrix} \mathbf{H_{11}} & 0 \\ \mathbf{H_{21}} & \mathbf{H_{22}} \end{pmatrix}, \mathbf{S} = \begin{pmatrix} \mathbf{0} & \mathbf{S_{12}} \\ 0 & \mathbf{S_{22}} \end{pmatrix},$$

$$\mathbf{\Psi}_1^T = (\psi_{\frac{1}{2},\frac{1}{2}}, \psi_{1,\frac{1}{2}}, \cdots, \psi_{K,\frac{1}{2}}, \psi_{K+\frac{1}{2},\frac{1}{2}}),$$

$$\begin{aligned}\mathbf{\Psi}_2^T = \ (\ & \psi_{\frac{1}{2},1}, \psi_{1,1}, \psi_{1,\frac{1}{2}}, \cdots, \psi_{K-\frac{1}{2},1}, \psi_{K,1}, \psi_{K,\frac{3}{2}}, \psi_{K+\frac{1}{2},1}, \\ & \cdots, \psi_{K-\frac{1}{2},N}, \psi_{K,N}, \psi_{K,N+\frac{1}{2}}, \psi_{K+\frac{1}{2},N}).\end{aligned}$$

$\mathbf{\Psi_1}$ denotes the fluxes in starting direction ($\mu = -1$) and $\mathbf{\Psi_2}$ describes the rest ones. $\mathbf{H_{i,j}}$ and $\mathbf{S_{i,j}}$ are block matrix elements, and detailed form can be deduced by Eqs. (3) (17) (18). We want to point out that even if not concrete structure of such matrixes, there exists $\mathbf{H^{-1}}$, because all fluxes can be explicitly obtained from the above solving procedure.

The purpose of this paper is to prove that the iterative solution of step function schemes (3)–(10) convergent to that of discrete ordinate equations (11) and (12).

Theorem 1. *Suppose that $0 \le c_k \le \sigma_k, f_k > 0$, for $k = 1, 2, \cdots, K$, then the sequence $\mathbf{\Psi^{(n)}}$ defined by schemes (3)-(10) with step function relationships (13) and (14) converge as $n \to \infty$, and the limit is independent of initial value $\mathbf{\Psi^{(0)}}$.*

2. Convergence of Inner Iterations Scheme

Before proving the Theorem 1, we state the following auxiliary lemmas:

Lemma 1 (See Theorem 2.7 in [6, pp. 46] or Corollary 5.2 in [7, pp. 37]). *If $\mathbf{A} \in R^{n\times n}$ is real and non-negative matrix, then spectral radius $\rho(\mathbf{A})$ is an eigenvalue of $\mathbf{A}$, and there exists a non-negative eigenvector of $\mathbf{A}$ associated with $\rho(\mathbf{A})$.*

Lemma 2 (see Theorem 1.4 in [6, pp. 13] or Theorem 1.1 in [7, pp. 113]). *Consider the stationary iterative method*

$$\psi^{(n+1)} = \mathbf{A}\psi^{(n)} + \mathbf{f}, \tag{15}$$

where $\mathbf{A} \in R^{n\times n}$, $\mathbf{f} \in R^n$. Then the method (15) is convergent if and only if $\rho(\mathbf{A}) < 1$.

Proof of Theorem 1.

For $\mu_m = -1$, substituting (9) into (8), we have

$$\psi_{k,\frac{1}{2}}^{(n+1)} = [A_{k+\frac{1}{2}}\psi_{k+\frac{1}{2},\frac{1}{2}}^{(n+1)} + S_k^{(n)}]/E_0 \tag{16}$$

where

$$E_0 = A_{k-\frac{1}{2}} + V_k\sigma_k.$$

So $\psi_{k,\frac{1}{2}}^{(n+1)} > 0, k = 1, 2, \cdots, K-1$, by the vacuum boundary condition (10).

Similarly, for $\mu_m < 0$, substituting (6) and (7) into (3), we have

$$\psi_{km}^{(n+1)} = [-\mu_m A_{k+\frac{1}{2}}\psi_{k+\frac{1}{2},m}^{(n+1)} + \frac{1}{\omega_m}(A_{k+\frac{1}{2}} - A_{k-\frac{1}{2}})\alpha_{m-\frac{1}{2}}\psi_{k,m-\frac{1}{2}}^{(n+1)} + S_k^{(n)}]/E_1 \tag{17}$$

where

$$E_1 = -\mu_m A_{k-\frac{1}{2}} + \frac{1}{\omega_m}(A_{k+\frac{1}{2}} - A_{k-\frac{1}{2}})\alpha_{m+\frac{1}{2}} + V_k\sigma_k.$$

For $\mu_m > 0$,

$$\psi_{km}^{(n+1)} = [\mu_m A_{k-\frac{1}{2}}\psi_{k-\frac{1}{2},m}^{(n+1)} + \frac{1}{\omega_m}(A_{k+\frac{1}{2}} - A_{k-\frac{1}{2}})\alpha_{m-\frac{1}{2}}\psi_{k,m-\frac{1}{2}}^{(n+1)} + S_k^{(n)}]/E_2 \tag{18}$$

where

$$E_2 = \mu_m A_{k+\frac{1}{2}} + \frac{1}{\omega_m}(A_{k+\frac{1}{2}} - A_{k-\frac{1}{2}})\alpha_{m+\frac{1}{2}} + V_k\sigma_k.$$

Under the given boundary and symmetry conditions (4)-(5), we can draw a conclusion $\psi_{km}^{(n+1)} \ge 0$. By (6) and (7) the iterative operation $\mathbf{H^{-1}S}$ is non-negative one.

Suppose that the iterative process is not convergent. From Lemmas 1 and 2, the matrix spectral radius $\rho \ge 1$ is an eigenvalue of solution operator $\mathbf{H^{-1}S}$, and the eigenvector is non-negative. Let $\lambda = 1/\rho \le 1$, then there is a non-negative vector $\psi_{km}, \psi_{k+\frac{1}{2},m}$ and $\psi_{k,m+\frac{1}{2}}$ such that

$$\mu_m(A_{k+\frac{1}{2}}\psi_{k+\frac{1}{2},m} - A_{k-\frac{1}{2}}\psi_{k-\frac{1}{2},m})$$

$$+(A_{k+\frac{1}{2}} - A_{k-\frac{1}{2}}) \cdot \frac{\alpha_{m+\frac{1}{2}}\psi_{k,m+\frac{1}{2}} - \alpha_{m-\frac{1}{2}}\psi_{k,m-\frac{1}{2}}}{\omega_m} \tag{19}$$

$$+V_k\sigma_k\psi_{km} = \lambda V_k c_k \sum_{j=1}^{N} \psi_{kj}\omega_j.$$

These $\psi_{km}, \psi_{k+\frac{1}{2},m}$ and $\psi_{k,m+\frac{1}{2}}$ satisfy the relations (4)-(10) with $f_k = 0$.

Multiplying (19) by ω_m, and summing over $1 \le m \le N$ and $1 \le k \le K$, we have

$$A_{K+\frac{1}{2}} \sum_{m=1}^{N} \mu_m\omega_m\psi_{K+\frac{1}{2},m} - A_{\frac{1}{2}} \sum_{m=1}^{N} \mu_m\omega_m\psi_{\frac{1}{2},m}$$

$$+\sum_{k=1}^{K}\sum_{m=1}^{N} V_k\sigma_k\omega_m\psi_{km} = \lambda \sum_{k=1}^{K}\sum_{m=1}^{N} V_k c_k\omega_m\psi_{km}. \tag{20}$$

Here we have used the fact that μ_m are even Gaussian sets, $\omega_m = \omega_{N-m+1}, \mu_m = -\mu_{N-m+1}$ for $m = 1, 2, \cdots, \frac{N}{2}$ and $\alpha_{N+\frac{1}{2}} = \alpha_{\frac{1}{2}} = 0$. Considering the vacuum boundary conditions (4) and symmetrical conditions (5) with respect to $m = 1, 2, \cdots, N/2$, there is

$$A_{K+\frac{1}{2}} \sum_{m=N/2+1}^{N} \mu_m\omega_m\psi_{K+\frac{1}{2},m} + \sum_{k=1}^{K}\sum_{m=1}^{N} V_k(\sigma_k - \lambda c_k)\omega_m\psi_{km} = 0.$$

Since $\sigma_k \ge c_k$, there is

$$\psi_{K+\frac{1}{2},m} = 0, \quad m = N/2+1, \cdots, N.$$

From the step function relations (13), there are

$$\psi_{K,m} = 0, \quad m = N/2+1, \cdots, N.$$

By use of non-negative feature of (19), (6)-(10) and (13)(14), we can obtain

$$\psi_{k,m} = 0, \quad k = 1, \cdots, K; \quad m = 1, \cdots, N$$

and $\psi_{k+\frac{1}{2},m} \equiv 0, \psi_{k,m+\frac{1}{2}} \equiv 0$. This contradicts that $\{\psi_{km}, \psi_{k+\frac{1}{2},m}, \psi_{k,m+\frac{1}{2}}\}$ is an eigenvector. The proof of the theorem is completed.

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