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CONVERGENCE OF INNER/OUTER SOURCE ITERATIONS WITH FINITE TERMINATION OF THE INNER ITERATIONS

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ABSTRACT. A two-stage (nested) iteration strategy, in which the outer iteration is analogous to a block Gauss-Seidel method and the inner iteration to a Jacobi method for each of these blocks, often are used in the numerical solution of discretized approximations to the neutron transport equation. This paper is concerned with the effect, within a continuous space model, of errors from finite termination of the inner iterations upon the overall convergence. The main result is that convergence occurs, to the solution of the original problem, in the limit that both the outer iteration index and the minimum over all outer indices and all groups ("blocks") jointly become large. Positivity properties (in the sense of cone preserving) are used extensively.

1. Introduction. A first step in computationally solving energy dependent linear (steady state) particle transport problems often is to introduce so-called *outer* (energy/group) source iteration. Conceptually, each step within this iteration involves solution of a sequence of monoenergetic transport problems. It is widespread practice to solve these by *inner* (direction) source iteration. This paper is concerned with the effect of the (computationally necessary) finite termination of the inner iterations upon the convergence of the approximations produced by the outer iterations. It is self-contained regarding the technical aspects of these iterative processes, but the interested reader is referred to the monographs by Bell and Glasstone [**1**], Duderstadt and Martin [**2**], Lewis and Miller [**3**], and Marchuk and Lebedev [**4**] for further background in transport theory.

Suppose that the underlying "exact" transport problem is subcritical (satisfies assumption A.4 of the next section), and denote the corresponding angular flux (the vector of dependent variables) by $\psi = \psi(x)$. If $\psi^{(i)} = \psi^{(i)}(x)$ denotes the ith approximation from the outer source iteration, then it is relatively easy (see §II for an example) to show that

$$\psi = \lim_{i\to\infty} \psi^{(i)}, \tag{1}$$

in some suitable sense. Similarly, if $\psi^{(i,j)}$ denotes the jth inner source iteration approximation to $\psi^{(i)}$, then one can readily show (see §III) that

$$\psi^{(i)} = \lim_{j\to\infty} \psi^{(i,j)}. \tag{2}$$

By combining (1) and (2), we have a presentation of the exact flux as an iterated limit,

$$\psi = \lim_{i\to\infty} \left\{ \lim_{j\to\infty} \psi^{(i,j)} \right\}. \tag{3}$$

Such presentations are the classical theoretical basis for the inner/outer source iteration procedure. However, this iterated limit neglects possible effects resulting from the fact that the inner iterations must be terminated at some finite value of j; e.g., it is conceivable that the error from this finite termination at each i could be small, while the cumulative effect of these overall i up to some I could become quite large as I increases. *The purpose of this paper is to address questions relating to how finite termination of the inner iterations affects the overall behavior of the iterative approximation.* The major result is Theorem 5.10 which asserts (roughly) that the approximations converge to the exact angular flux as both the number of outer iterations and minimum number of inner iterations (over all groups and outer iterations) jointly approach infinity.

For definiteness we carry out the present study in the context of the spatially continuous discrete-ordinate multigroup model of (linear) particle transport in plane-parallel geometry. It appears that the results and techniques would readily carry over to models incorporating continuous direction or energy. However, note that it seems to be a rather more delicate matter to analyze interactions between source iteration and spatial discretizations. Refer to Menon and Sahni [**5**] and Nelson [**6**] for some recent results in that regard, along with references to earlier related works.

In §II we set the notation and establish a precise version of (1). §III similarly is devoted to obtaining a precise version of (2). §IV is devoted to establishing conditions under which the iterated limit in (3) can be replaced by the corresponding double limit. More complex arguments are used in §V to prove the major result described above. The concluding §VI is devoted primarily to suggestions for further related studies.

We conclude this introduction by briefly reviewing previous convergence results for two-stage linear iterative procedures. See Golub and Overton [**7,8**] and the fundamental paper of Nichols [**9**], along with further works cited in these references, for such results in a finite-dimensional setting. Dupont [**10**] has obtained similar results for positive-definite operator equations and a specific two-stage iteration. None of these earlier works use the monotonicity properties (based on positivity in the sense of order-preserving) that are the cornerstone of the following results.

2. Outer source iteration. For arbitrary fixed positive G and M, let $\mathcal{G} := \{(g,m) : g = 1,\ldots,G,\ m = 1,\ldots,M\}$. Then write the discrete-ordinate multigroup transport equation in plane-parallel geometry as the linear system of ordinary differential equations

$$\mu_m \frac{d\psi_{gm}}{dx} + \sigma_g \psi_{gm} = (\mathbf{K}\psi)_{gm} + q_{gm}, \quad (g,m) \in \mathcal{G}, \tag{4}$$

where $\psi = \{\psi_{gm} : (g,m) \in \mathcal{G}\}$ and

$$(\mathbf{K}\psi)_{gm}(x) := \sum_{(g',m') \in \mathcal{G}} k_{gmg'm'}(x)\psi_{g'm'}(x),\ (g,m) \in \mathcal{G}. \tag{5}$$

Here ψ_{gm} is the angular flux for energy group g in the directions specified by direction cosine μ_m, and the remaining symbols represent various given quantities in more or less standard notation.

In the present work consider (4) and (5) subject only to boundary conditions representing known incident flux,

$$\begin{aligned} \psi_{gm}(0) &= \beta_{gm}, \text{ for } (g,m) \in \mathcal{G} \text{ and } \mu_m > 0, \\ \psi_{gm}(a) &= \beta_{gm}, \text{ for } (g,m) \in \mathcal{G} \text{ and } \mu_m < 0, \end{aligned} \tag{6}$$

where a is some positive number. However, it appears likely that the basic results can be extended to more general (linear) boundary conditions.

As regards the data for the two-point boundary-value problem (4) – (6), we make the following assumptions:

A.1. For each $m = 1, \ldots, M$, $\mu_m \in [-1,1] \sim \{0\} \equiv [-1,0) \cup (0,1]$.

A.2. The β_{gm} are nonnegative constants, for $(g,m) \in \mathcal{G}$.

A.3. The $\{\sigma_g\}, \{q_{gm}\}$ and $\{k_{gmg'm'}\}$ are nonnegative piecewise continuous functions on $[0,a]$, for each (g,m) and (g',m') in $\mathcal{G}$.

Let $\mathcal{C}$ denote the set of continuous real-valued functions, defined on $[0,a]$. Further, let $\mathcal{PC}$ be the set of real-valued functions defined on $[0,a]$ that are continuous except for jump discontinuities at one of the finitely many discontinuities σ_g, q_{gm} or $k_{gmg'm'}$. Regard $\mathcal{C}^{\mathcal{G}}, \mathcal{PC}^{\mathcal{G}}, \mathcal{C}^M$ and $\mathcal{PC}^M$ as Banach spaces. The norm associated with $\mathcal{C}^{\mathcal{G}}$ is sup over all $x \in [0,a], m = 1, \ldots, M$ and $g = 1, \ldots, G$. The norm associated with the other spaces is the sup norm over all $x \in [0,a]$ and all $m = 1, 2, \ldots, M$. The following is a basic concept of our work.

DEFINITION 2.1. By a *solution* of the two-point boundary-value problem (TPBVP) (4) – (6) is meant an element $\psi = \{\psi_{gm}\}$ of $\mathcal{C}^{\mathcal{G}}$ such that the derivative of each ψ_{gm} exists on $[0,a]$, again except possibly at finitely many points, and, further, the $\{\psi_{gm}\}$ satisfy the boundary conditions (6).

With this understanding of solution, we can formulate the following precise version of the subcriticality assumption:

A.4. For any *boundary fluxes* $\{\beta_{gm}\}$ and *source function* $\{q_{gm}\}$, as in assumption **A.2** and **A.3**, respectively, the TPBVP (4) – (6) has a unique solution, and further that solution is nonnegative. (To say that $\psi = \{\psi_{gm}\}$ is nonnegative means that each ψ_{gm} assumes only nonnegative values.)

Throughout the remainder of this work we suppose, without explicitly noting, that assumptions **A.1** – **A.4** hold. We define $\mathbf{S} : \mathcal{PC}^{\mathcal{G}} \to \mathcal{C}^{\mathcal{G}}$ by

$$(7) \qquad (\mathbf{S}f)_{gm}(x) = \int_{a_m}^{x} \frac{1}{\mu_m} \exp\Big\{ -\frac{1}{\mu_m} \int_{x'}^{x} \sigma_g(s)\,ds \Big\} f_{gm}(x')\,dx',$$

where

$$a_m = \begin{cases} 0, & \mu_m > 0, \\ a, & \mu_m < 0. \end{cases}$$

In the ensuing we need the following easily proved result.

PROPOSITION 2.2. *An element* $\psi = \{\psi_{gm}\}$ *of* $C^{\mathcal{G}}$ *is a solution of the* TPBVP (4) – (6) *if and only if it satisfies*

$$\psi = \mathbf{SK}\psi + Sq + b, \tag{8}$$

where $q := \{q_{gm} : (g,m) \in \mathcal{G}\} \in \mathbf{P}C^{\mathcal{G}}$ *and* $b \in C^{\mathcal{G}}$ *has components*

$$b_{gm} = \beta_{gm} \exp\Big\{ -\frac{1}{\mu_m} \int_{a_m}^{x} \sigma(s)\, ds \Big\}. \tag{9}$$

REMARK 2.3. It should be clear from **A.3** that $\mathbf{K}(C^{\mathcal{G}}) \subset \mathcal{P}C^{\mathcal{G}}$ where $\mathbf{K}$ is as defined by (5). Hence $\mathbf{SK} : C^{\mathcal{G}} \to C^{\mathcal{G}}$.

With the preceding preliminary technical matters in hand, we turn now to a precise formulation of the outer source iteration. Toward that end let the operators $\mathbf{L}, \mathbf{D}$ and $\mathbf{U}$ be defined by

$$(\mathbf{L}f)_{gm} := \sum_{g'=1}^{g-1} \sum_{m'=1}^{M} k_{gmg'm'} f_{g'm'}, \quad (g,m) \in \mathcal{G},$$

$$(\mathbf{D}f)_{gm} := \sum_{m'=1}^{M} k_{gmgm'} f_{gm'}, \quad (g,m) \in \mathcal{G},$$

and

$$(\mathbf{U}f)_{gm} := \sum_{g'=g+1}^{G} \sum_{m'=1}^{M} k_{gmg'm'} f_{g'm'}, \quad (g,m) \in \mathcal{G}.$$

As in Remark 2.3, it should be clear that each of $\mathbf{L}, \mathbf{D}$ and $\mathbf{U}$ map $C^{\mathcal{G}}$ into $\mathcal{P}C^{\mathcal{G}}$. It further should be clear that

$$\mathbf{K} = \mathbf{L} + \mathbf{D} + \mathbf{U}. \tag{10}$$

The outer source iteration is then formally defined by

$$(\mathbf{I} - \mathbf{SD} - \mathbf{SL})\psi^{(i+1)} = \mathbf{SU}\psi^{(i)} + \mathbf{S}q + b, \tag{11}$$

$$\psi^{(0)} = 0, \tag{12}$$

where the parenthetical superscript is an iteration index and $\mathbf{I}$ is the identity operator on $\mathcal{C}^{\mathcal{G}}$. The formality resides in the fact that we have not yet established invertibility of $\mathbf{I} - \mathbf{S}(\mathbf{D} + \mathbf{L})$. The following result is the first step toward remedying this situation.

THEOREM 2.4. *The operator* $(\mathbf{I} - \mathbf{SK})^{-1}$ *exists as a bounded linear operator on* $\mathcal{C}^{\mathcal{G}}$ *(into itself), and, further,*

$$(\mathbf{I} - \mathbf{SK})^{-1} = \sum_{n=0}^{\infty} (\mathbf{SK})^n, \tag{13}$$

where the (Neumann) series on the right converges in the operator norm on $\mathcal{C}^{\mathcal{G}}$.

PROOF. Let β and q satisfy A.2 and A.3 respectively, and let ψ be the corresponding solution of (4) – (6) (nonnegative and unique within $\mathcal{C}^{\mathcal{G}}$) that exists by **A.4**. By Proposition 2.2 and adroit use of (8) we find

$$\sum_{n=0}^{N} (\mathbf{SK})^n (\mathbf{S}q + b) \le \psi = \sum_{n=0}^{N} (\mathbf{SK})^n (\mathbf{S}q + b) + (\mathbf{SK})^{N+1}\psi,$$

where henceforth order relations between elements of $\mathcal{C}^{\mathcal{G}}$ are to be interpreted componentwise. This implies that

$$\sum_{n=0}^{\infty} [(\mathbf{SK})^n (\mathbf{S}q + b)](x)$$

converges for each x in $[0, a]$. Similarly

$$\sum_{n=0}^{\infty} [(\mathbf{SK})^n f](x) \tag{14}$$

converges to a finite-valued integrable function for each nonnegative f in $\mathcal{C}^{\mathcal{G}}$ (and hence each f in $\mathcal{C}^{\mathcal{G}}$) and all such x, as can be seen by bounding such f above by suitable $\mathbf{S}q + b$.

Next we claim the convergence of (14) is uniform in $x \in [0, a]$ for such nonnegative f in $\mathcal{C}$, and for all f in $\mathcal{C}$. In order to see this, let (14) be denoted $F(x)$. The monotone convergence theorem gives

$$\mathbf{SK}F(x) = \sum_{n=0}^{\infty}[(\mathbf{SK})^{n+1}f](x) = F(x) - f(x). \tag{15}$$

Here we have temporarily extended the respective definitions (5) and (7) of $\mathbf{K}$ and $\mathbf{S}$ to MG-tuples of finite-valued integrable functions, as essentially that is all that is *a priori* known of F. However, $\mathbf{SK}$ maps any such MG-tuple into an element of $\mathcal{C}^{\mathcal{G}}$, and so (15) itself shows $F \in \mathcal{C}^{\mathcal{G}}$. The desired uniform convergence then follows from monotonicity of (14) along with Dini's theorem.

We now know that the right-hand side of (13) converges strongly in $\mathcal{C}^{\mathcal{G}}$. That this pointwise limit is bounded follows from the principle of uniform boundedness, and that it is $(\mathbf{I} - \mathbf{SK})^{-1}$ follows from computations similar to those leading to (15). Uniform (i.e., operator norm) convergence of (13) then follows from the fact that uniform and strong convergence of Neumann series are equivalent, which in turn is a consequence of the well-known fact (e.g., Theorem 3.10.1 of Hille and Phillips [**11**]) that uniform and strong analyticity are equivalent for operator-valued functions. □

COROLLARY 2.5. *Under the assumptions of Theorem* 2.4, $(\mathbf{I}-\mathbf{SK})^{-1}$ *is a positive operator in the sense that it maps nonnegative elements of* $\mathcal{C}^{\mathcal{G}}$ *into such elements.*

PROOF. This follows from (13) and the fact that each of $\mathbf{S}, \mathbf{K}$ are positive operators. □

COROLLARY 2.6. *The operator* $[\mathbf{I} - \mathbf{S}(\mathbf{D} + \mathbf{L})]^{-1}$ *exists as a positive bounded linear operator on* $\mathcal{C}^{\mathcal{G}}$ *into itself, and, further,*

$$[\mathbf{I} - \mathbf{S}(\mathbf{D} + \mathbf{L})]^{-1} = \sum_{n=0}^{\infty}[\mathbf{S}(\mathbf{D} + \mathbf{L})]^n, \tag{16}$$

where the Neumann series on the right-hand side of (16) *converges uniformly (i.e., in the operator norm on* $\mathcal{C}^{\mathcal{G}}$*).*

PROOF. For each nonnegative $f \in \mathcal{C}^{\mathcal{G}}$,

$$\sum_{n=0}^{\infty}\{[\mathbf{S}(\mathbf{D}+\mathbf{L})^n f\}(x)$$

converges, as can be seen by comparison with (14). The remainder of the proof essentially is identical to the latter two-thirds of the proof of Theorem 2.4. □

Corollary 2.6 assures that the outer iteration process is well-posed, in the sense that all iterates exist. The following, which has been the ultimate aim of this section, insures that these iterates converge to the solution of the TPBVP (1) – (3).

THEOREM 2.7. *The* $\{\psi^{(i)}\}$, *as defined by* (11) *and* (12), *converge in* $\mathcal{C}^{\mathcal{G}}$ *to the solution of the* TPBVP (4) – (6) *as* $i \to \infty$.

PROOF. If ψ is the solution of (4) – (6), then a simple induction proof shows that $0 \leq \psi^{(i)} \leq \psi^{(i+1)} \leq \psi$. Application of the monotone convergence theorem to (11) shows that $\hat{\psi} = \mathbf{SK}\hat{\psi} + \mathbf{S}q + b$, where $\hat{\psi}$ is the pointwise limit of the $\psi^{(i)}$. But $\hat{\psi} = \psi$ then follows from the subcriticality assumption (A.4) and Proposition 2.2. □

In practice one often initiates the outer source iteration not by (12), but by some other $\psi^{(0)}$ thought to be a better approximation to ψ. As far as convergence *per se* is concerned, the following result shows that the choice of $\psi^{(0)}$ is immaterial.

COROLLARY 2.8. *The sequence* $\{\psi^{(i)}\}$, *as defined by* (12), *converges in* $\mathcal{C}^{\mathcal{G}}$ *to the solution of the* TPBVP (1) – (3) *as* $i \to \infty$, *for arbitrary* $\psi^{(0)}$ *in* $\mathcal{C}^{\mathcal{G}}$.

PROOF. If $\psi^{(0)} = 0$, then it is easy to compute

$$\psi^{(i)} = \sum_{n=0}^{i-1}\mathbf{Q}^n(\mathbf{S}q + b),$$

where

$$\mathbf{Q} := [\mathbf{I} - \mathbf{S}(\mathbf{D} + \mathbf{L})]^{-1}\mathbf{S}\mathbf{U}.$$

Therefore the conclusion of Theorem 2.7 can be reformulated as

$$\psi = \sum_{n=0}^{\infty} \mathbf{Q}^n(\mathbf{S}q + b). \tag{17}$$

If the iteration begins with arbitrary $\psi^{(0)}$, then the corresponding ith iterate is readily computed as

$$\psi^{(i)} = \sum_{n=0}^{i-1} \mathbf{Q}^n(\mathbf{S}q + b) + \mathbf{Q}^i\psi^{(0)}.$$

But we have shown that (17) converges for arbitrary q and b, subject to **A.2** and **A.3**. By picking these sufficiently large so as to dominate $\psi^{(0)}$, we conclude that $\mathbf{Q}^i\psi^{(0)} \to 0$ (in $\mathcal{C}^{\mathcal{G}}$) as $i \to \infty$. It follows that

$$\lim_{i\to\infty} \psi^{(i)} = \sum_{n=0}^{\infty} \mathbf{Q}^n(\mathbf{S}q + b) = \psi.$$

This completes both the proof of Corollary 2.8 and §II. □

3. Inner source iteration. In order to implement the outer source iteration scheme described in the preceding section, it is necessary to solve the linear system (11) of integral equations for each $\psi^{(i+1)}$, given $\psi^{(i)}$. The basic purpose of this section is to show that this can be accomplished by the so-called inner source iteration scheme. Prior to defining this scheme and developing its properties, further notation is required.

For each $g = 1, \ldots, G$, define $\mathbf{P}_g : \mathcal{PC}^{\mathcal{G}} \to \mathcal{PC}^M$ by

$$\mathbf{P}_g f = \{f_{gm} : m = 1, \ldots, M\}, \tag{18a}$$

where $f = \{f_{g'm} : (g', m) \in \mathcal{G}\}$. Similarly, for each $m = 1, \ldots, M$, define $\hat{\mathbf{P}}_m : \mathcal{PC}^M \to \mathcal{PC}$ by

$$\hat{\mathbf{P}}_m f = f_m, \tag{18b}$$

where now $f = \{f_{m'} : m' = 1, \dots, M\}$. For $f \in \mathcal{PC}^{\mathcal{G}}(\mathcal{PC}^M)$ we shall often denote $\mathbf{P}_g f$ and $\hat{\mathbf{P}}_m \mathbf{P}_g f(\hat{\mathbf{P}}_m f)$ respectively by f_g and $f_{gm}(f_m)$, with or without modifiers (e.g., primes) on the generic subscripts. We shall also denote the restriction of $\mathbf{P}_g(\hat{\mathbf{P}}_m)$ to $\mathcal{C}^{\mathcal{G}}(\mathcal{C}^M)$ by $\mathbf{P}_g(\hat{\mathbf{P}}_m)$. For such $g,\ g' = 1, \dots, G$ with $g' < g$ (respectively $g' = g,\ g' > g$) define the operator $L_{gg'}(D_{gg'}, U_{gg'})$ mapping $\mathcal{C}^M$ onto $\mathcal{PC}^M$ by

$$(19) \qquad \begin{aligned} &(L_{gg'} f)_m(x)((D_{gg} f(x))_m, (U_{gg'} f(x))_m) \\ &:= \sum_{m'=1}^{M} k_{gmg'm'}(x) f_{g'm'}(x). \end{aligned}$$

Further define $\mathbf{S}_g : \mathcal{PC}^M \to \mathcal{C}^M$, for each $g = 1, \dots, G$, by

$$(\mathbf{S}_g f)_m = \frac{1}{\mu_m} \int_{a_m}^{x} \exp\left\{ -\frac{1}{\mu_m} \int_{x'}^{x} \sigma_g(s)\, ds \right\} f_m(x')\, dx',$$

where $f = \{f_m : m = 1, \dots, M\} \in \mathcal{C}^M$.

With these matters of notation in hand, first note that the result of acting upon (11) by $\mathbf{P}_g$ can be written

$$(20) \qquad \begin{aligned} (\mathbf{I}_M - \mathbf{S}_g \mathbf{D}_{gg})\psi_g^{(i+1)} = \mathbf{S}_g &\left[\sum_{g'=1}^{g-1} \mathbf{L}_{gg'} \psi_{g'}^{(i+1)} + \sum_{g'=g+1}^{G} \mathbf{U}_{gg'} \psi_{g'}^{(i)} \right] \\ &+ \mathbf{S}_g q_g + b_g, \end{aligned}$$

where $\mathbf{I}_M$ is the identity operator on $\mathcal{C}^M$. Now if the $\psi_g^{(i+1)}$ can be determined in the order of increasing values of g, that is $g = 1, \dots, G$, then, at each fixed value of g, the right-hand side of (20) is known. Therefore, we momentarily focus attention upon systems of the form

$$(21) \qquad (\mathbf{I}_M - \mathbf{S}_g \mathbf{D}_{gg})\varphi = h,$$

where $h \in \mathcal{C}^M$ is known. If $h = \mathbf{S}_g q_g + b_g$, then it should be clear that (21) is equivalent to the TPBVP consisting of the *monoenergetic* (discrete-ordinates) transport equation with source functions equal to the components of q_g and boundary data equal to the components of β_g.

REMARK. Usually increasing values of the index g correspond to decreasing group energies; however, this condition plays no role in our convergence studies. It usually will play a role in the *rate* of convergence, and indeed it is a fact that the $U_{gg'}$ often have small norm if increasing g does correspond to decreasing energy that suggests the outer iteration scheme.

THEOREM 3.1. *Each* $(\mathbf{I}_M - \mathbf{S}_g\mathbf{D}_{gg})^{-1}$ *exists as a bounded linear operator on* $\mathcal{C}^M$ *into itself, and, further,*

$$(\mathbf{I}_M - \mathbf{S}_g\mathbf{D}_{gg})^{-1} = \sum_{n=0}^{\infty}(\mathbf{S}_g\mathbf{D}_{gg})^n, \tag{22}$$

where the Neumann series on the right converges in the operator norm on $\mathcal{C}^M$. *Therefore,* $(\mathbf{I}_M - \mathbf{S}_g\mathbf{D}_{gg})^{-1}$ *is a positive operator on* $\mathcal{C}_M$.

PROOF. Let h be an arbitrary given nonnegative element of $\mathcal{C}^M$. For such h, let $\hat{h} = \mathbf{S}_g q_g + b_g$, where q_g and b_g are selected so that $h \leq \hat{h}$. Consider the outer iteration scheme (12) with source functions

$$q_{g'} = \begin{cases} q_g & \text{if } g' = g, \\ 0 & \text{otherwise,} \end{cases}$$

boundary data $\beta_{g'm}$ as defined by b_g (in $\hat{h}$) if $g' = g$, $\beta_{g'm} = 0$ otherwise, and initial approximation $\psi^{(0)} = 0$. By the results of the preceding section (applied to the system modified by setting $L_{gg'} = U_{gg'} \equiv 0$), the system

$$(\mathbf{I}_M - \mathbf{S}_g\mathbf{D}_{gg})\hat{\psi} = \hat{h}$$

has a unique solution, say $\psi_g^{(1)}$, and, further, $\psi_g^{(1)}$ is nonnegative. By employing Dini's theorem as in the proof of Theorem 2.4, we conclude that the Neumann series

$$\sum_{n=0}^{\infty}(\mathbf{S}_g\mathbf{D}_{gg})^n\hat{h}$$

converges in C. By majorization the Neumann series

$$\sum_{n=0}^{\infty}(\mathbf{S}_g\mathbf{D}_{gg})^n h$$

likewise converges for each fixed $x \in [0, a]$, and by again employing Dini's Theorem this convergence actually is uniform in $\mathcal{C}^M$. Again, as in the proof of Theorem 2.4, this strong convergence actually implies uniform convergence. That the limit actually is $(\mathbf{I}_M - \mathbf{S}_g\mathbf{D}_{gg})^{-1}$ simply is a matter of straightforward calculation, as that which yielded (15) above. □

For each $g = 1, \ldots, G$ let $\hat{\mathbf{D}}_g$ and $\overline{\mathbf{D}}_g$, both mapping $\mathcal{C}^M$ into $\mathcal{PC}^M$, be defined respectively by

$$\hat{\mathbf{P}}_m\hat{\mathbf{D}}_g f(x) = k_{gmgm}(x) f_m(x)$$

and

$$\hat{\mathbf{P}}_m\overline{\mathbf{D}}_g f(x) = \sum_{\substack{m'=1 \\ m'\neq m}}^{m} k_{gmgm'} f_{m'}(x).$$

The inner source iteration for a system of the form (21) then is defined by

$$(23) \qquad (\mathbf{I}_M - \mathbf{S}_g\hat{\mathbf{D}}_g)\varphi^{(j+1)} = \mathbf{S}_g\overline{\mathbf{D}}_g\varphi^{(j)} + h.$$

The following result establishes that this iteration process is well-defined:

THEOREM 3.2. *Each $(\mathbf{I}_M - \mathbf{S}_g\hat{\mathbf{D}}_g)^{-1}$, for $g = 1, \ldots, G$, exists as a bounded linear operator, and, further, is given by*

$$(24) \qquad (\mathbf{I}_M - \mathbf{S}_g\hat{\mathbf{D}}^g)^{-1} = \sum_{n=0}^{\infty}(\mathbf{S}_g\hat{\mathbf{D}}_g)^n,$$

where the Neumann series on the right converges in the operator norm on $\mathcal{C}^M$; in particular each $(\mathbf{I}_m - \mathbf{S}_g\hat{\mathbf{D}}_g)^{-1}$ is a positive operator on $\mathcal{C}^M$.

PROOF. This result follows immediately from Theorem 3.1, along with the fact that the Neumann series in (24) is termwise dominated by that in (22). □

Our next result establishes that the sequence produced by an inner source iteration (23) converges to the solution of (21), for arbitrary starting values.

THEOREM 3.3. *For each* $g = 1, \dots, G$ *the* $\{\varphi^{(j)}\}$, *as defined by* (23) *with arbitrary starting value* $\varphi^{(0)} \in \mathcal{C}^M$, *converge in* $\mathcal{C}^M$ *to the solution of* (21).

PROOF. It suffices to establish the result for nonnegative h. If $\varphi = (\mathbf{I}_M - \mathbf{S}_g\mathbf{D}_{gg})^{-1}h = \sum_{n=0}^{\infty}(\mathbf{S}_g\mathbf{D}_{gg})^n h$ is the solution of (21) and $\varphi^{(0)} = 0$, then $0 = \varphi^{(0)} \leq \varphi$, which, with the result of Theorem 3.2, implies

$$\begin{aligned} 0 = \varphi^{(0)} \leq \varphi^{(1)} &= (\mathbf{I}_M - \mathbf{S}_g\hat{\mathbf{D}}_g)^{-1}[\mathbf{S}_g\hat{\mathbf{D}}_g\varphi^{(0)} + h] \\ &\leq (\mathbf{I}_M - \mathbf{S}_g\hat{\mathbf{D}}_g)^{-1}[\mathbf{S}_g\hat{\mathbf{D}}_g\varphi + h] = \varphi. \end{aligned}$$

If we assume that

$$0 \leq \varphi^{(j)} \leq \varphi^{(j+1)} \leq \varphi, \tag{25}$$

then similarly we can establish that $0 \leq \varphi^{(j+1)} \leq \varphi^{(j+2)} \leq \varphi$, which inductively establishes (25) for all $j = 1, 2, \dots$. The proof that the $\varphi^{(j)}$ converge to φ essentially is the same as that of Theorem 2.7, and the extension to arbitrary starting values is as in the proof of Corollary 2.8. We omit the details. □

The inner source iteration for the outer approximation $\varphi_g^{(i+1)}$ is defined by

$$(\mathbf{I}_M - \mathbf{S}_g\hat{\mathbf{D}}_g)\psi_g^{(i+1,j+1)} = \mathbf{S}_g\overline{\mathbf{D}}_g\psi_g^{(i+1,j)} + h_g^{(i+1)}, \tag{26}$$

where

$$h_g^{(i+1)} := \mathbf{S}_g\Big[\sum_{g'=1}^{g-1}\mathbf{L}_{gg'}\psi_{g'}^{(i+1)} + \sum_{g'=g+1}^{G}\mathbf{U}_{gg'}\psi_{g'}^{(i)}\Big] + \mathbf{S}_g q_g + b_g \tag{27}$$

and the starting value

$$\psi_g^{(i+1,0)} := \psi_g^{(i)} \tag{28}$$

is used. Note that (26) and (27) are equivalent to the uncoupled system of scalar initial-value problems comprised of

$$\mu_m \frac{\partial\psi_{gm}^{(i+1,j+1)}}{\partial x} + \sigma_g(x)\psi_{gm}^{(i+1,j+1)} = w_{gm}^{(i,j)}, \quad m = 1, \dots, M,$$

and the obvious initial value obtained from (6), where

$$w_{gm}^{(i,j)} = \sum_{\substack{m'=1 \\ m'\neq m}}^{M} k_{gmgm'}(x)\psi_{gm'}^{(i+1,j)} + \hat{\mathbf{P}}_m\Big[\sum_{g'=1}^{g-1} \mathbf{L}_{gg'}\psi_{g'}^{(i+1)} + \sum_{g'=g+1}^{G} \mathbf{U}_{gg'}\psi_{g'}^{(i)}\Big] + q_{gm}$$

is known. Thus implementation of the inner iterations requires only the ability to solve a scalar initial-value problem. This almost invariably is done via some type of finite-difference method, although the imbedding of these initial-value problems within the source iteration imposes some additional requirement above those usually encountered in numerically solving initial-value problems by finite differences (cf. Nelson and Zelazny [**12**], Nelson [**13**], and Keller and Nelson [**14**] for more detailed discussions of such matters).

Let $\psi^{(i,j)} \in \mathcal{C}^{\mathcal{G}}$ be defined by the inner iteration scheme (26), (27), with arbitrary starting values $\psi_g^{(i,0)} \in \mathcal{C}^M$, where the outer iteration scheme (11) is initiated with arbitrary $\psi^{(0)} \in \mathcal{C}^{\mathcal{G}}$. It follows from Corollary 2.8 and Theorem 3.3 that the solution (ψ) of the TPBVP (4) – (6) is given by the iterated limit (3), where the limits are to be understood in the sense of the norm on $\mathcal{C}$. We next explore the possibility of replacing this iterated limit by the more general double limit.

4. Joint convergence results. A standard result of mathematical analysis is that existence of an iterated limit of a sequence (of real numbers) implies existence of the corresponding double limit (and thus equality of the two limits) if either the elements of the sequence are suitably monotone, or the convergence in the inner limit is uniform relative to the parameter in the outer limit. In this section we obtain results corresponding to this, for the double sequence defined by the inner/outer source iteration processes defined in the preceding two sections. The result using uniformity (Theorem 4.2) actually contains that involving monotonicity (Proposition 4.1); however, we choose to include the latter because its proof is somewhat simpler and because the form of this monotonicity, and the conditions insuring it, may be of independent interest.

Begin by considering $\psi^{(i,j)}$, as defined in the final paragraph of the preceding section, but with the specific starting values

$$\psi^{(0)} = 0 \tag{29a}$$

for the outer iteration and

$$\psi_g^{(i,0)} = 0, \; i \geq 1, \quad g = 1, \ldots, G, \tag{29b}$$

for the inner iterations. As already noted in the proof of Theorem 2.7, $\psi^{(i)} \leq \psi^{(i')}$ for $i \leq i'$. It follows that $i \leq i'$ implies $h_g^{(i)} \leq h_g^{(i')}$, where the latter are as in (27). But it is readily seen that

$$\psi_g^{(i,j)} = \sum_{n=0}^{j-1} [(\mathbf{I}_M - \mathbf{S}_g\hat{\mathbf{D}}_g)^{-1}\mathbf{S}_g\overline{\mathbf{D}}_g]^n (\mathbf{I}_M - \mathbf{S}_g\hat{\mathbf{D}}_g)^{-1} h_g^{(i)}.$$

From this representation, and positivity of $(\mathbf{I}_M - \mathbf{S}_g\hat{\mathbf{D}}_g)^{-1}$ (cf. Theorem 3.2) and $\mathbf{S}_g\overline{\mathbf{D}}_g$, it follows that if $(i,j) \leq (i',j')$ in the *product order* (i.e., $1 \leq i \leq i'$ *and* $0 \leq j \leq j'$), then $\psi_g^{(i,j)} \leq \psi^{(i',j')}$. It then follows that

$$\psi\left(:= \lim_{i\to\infty} \left\{ \lim_{j\to\infty} \psi^{(i,j)} \right\} \right) = \sup_{i,j} \psi^{(i,j)},$$

and thence it is straightforward to complete the proof of

PROPOSITION 4.1. *If* $\{\psi^{(i,j)}\}$ *is defined by the inner source iterations* (26) *and* (27), *with starting values given by* (29b), *and by the outer source iteration* (11), *with starting value* (29a), *then*

$$\lim_{i,j\to\infty} \psi^{(i,j)} = \psi, \tag{30}$$

where ψ *is the solution of the* TPBVP (4) – (6), *and further this limit is approached monotonically relative to the product order on pairs of iteration indices.*

This result is, insofar as the double limit (30) is concerned, subsumed in

THEOREM 4.2. *Let $\{\psi^{(i,j)}\}$ be defined by the outer source iteration* (11), *with arbitrary starting value $\psi^{(0)} \in \mathcal{C}$, and the inner source iteration* (26) *and* (27), *with starting values $\psi_g^{(i,0)} \in \mathcal{C}_M$ such that there exists a real number α such that*

$$\|\psi_g^{(i,0)}\|_M \leq \alpha, \quad 1 \leq i, \ g = 1, \ldots, G.$$

If ψ is the solution of the TPBVP (4) – (6), *then the $\psi^{(i,j)}$ tend to ψ in the sense of the limit* (30).

PROOF. Given $\varepsilon > 0$, we must show there exists I and J such that $i \geq I$ and $j \geq J$ imply

$$\max_{1 \leq g \leq G} \|\psi_g^{(i,j)} - \psi_g\| \leq \varepsilon.$$

As we know that

$$\psi = \lim_{i \to \infty} \psi^{(i)} \quad \text{(Corollary 2.8)},$$

where

$$\psi_g^{(i)} = \lim_{j \to \infty} \psi_g^{(i,j)} \quad \text{(Corollary 3.3)},$$

we may choose I so that $i \geq I$ implies

$$\max_{i \leq g \leq G} \|\psi - \psi^{(i)}\| \leq \varepsilon/2. \tag{31}$$

It is readily shown that

$$\begin{aligned} \psi_g^{(i)} - \psi_g^{(i,j)} = & \sum_{n=j}^{\infty} [(\mathbf{I}_M - \mathbf{S}_g \hat{\mathbf{D}}_g)^{-1} \mathbf{S}_g \overline{\mathbf{D}}_g]^n (\mathbf{I}_M - \mathbf{S}_g \hat{\mathbf{D}}_g)^{-1} h_g^{(i)} \\ & - [(\mathbf{I}_M - \mathbf{S}_g \hat{\mathbf{D}}_g)^{-1} \mathbf{S}_g \overline{\mathbf{D}}_g]^j \psi_g^{(i)}. \end{aligned} \tag{32}$$

But each $\{\psi_g^{(i)}\}_{i=1}^{\infty}$ is convergent and thus bounded; (27) then shows there exists B such that $\|\psi_g^{(i)}\| \leq B$ and $\|(\mathbf{I}_M - \mathbf{S}_g \hat{\mathbf{D}}_g)^{-1} h_g^{(i)}\| \leq B$, both for $i \geq 1$ and $G \geq g \geq 1$. Further, Theorem 3.3 implies that $r_\sigma[(\mathbf{I}_M - \mathbf{S}_g \hat{\mathbf{D}}_g)^{-1} \mathbf{S}_g \overline{\mathbf{D}}_g] < 1$ for each g such that $1 \leq g \leq G$, where

r_σ denotes spectral radius. It follows that there exists γ satisfying $0 \le \gamma < 1$ and N such that if $n \ge N$ then $\|[(\mathbf{I}_M - \mathbf{S}_g\hat{\mathbf{D}}_g)^{-1}\mathbf{S}_g\overline{\mathbf{D}}_g]^n\| \le \gamma^n$. If $j \ge N$, then (32) yields the estimate

$$\|\psi_g^{(i)} - \psi_g^{(i,j)}\| \le \sum_{n=j}^{\infty} \gamma^n B + \gamma^j B = B\gamma^j\Big\{1 + \frac{1}{1-\gamma}\Big\}.$$

But the expression on the right-hand side of this equality is bounded above by $\varepsilon/2$ if

$$j \ge \ln\Big[\frac{\varepsilon}{2\beta}\Big(\frac{1-\gamma}{2\gamma}\Big)\Big]\Big/\ln\gamma. \tag{33}$$

Therefore, if J is not less than either N or the right-hand side of (33), then $i \ge I$ and $j \ge J$ imply $\|\psi_g^{(i,j)} - \psi_g\|_M \le \varepsilon$, for $g = 1, \ldots, G$. This completes both the proof of Theorem 4.2 and §IV. □

5. Convergence with finite termination of inner iterations. The joint convergence result of the preceding section only *partially* takes into account termination of the inner source iterations at some finite point, in that it is based on data (i.e., $h_g^{(i)}$) for the inner iterations at the ith outer iteration level that assume the inner iterations at the preceding outer iteration levels have been carried to completion (cf. Equation (27)). In this section we establish results (Theorems 5.7 and 5.10) that remedy this defect; these results constitute the primary objective of the research reported here.

We begin by assuming that the inner iterations are terminated at the same step, say $\overline{j}$, for all groups and outer iteration levels. (This restriction will be relaxed below, but in fact it does correspond to a strategy that has been used in some production codes, e.g., DIF3D-T, cf. [**15**, p. 4-8]). Let the corresponding approximation to the angular flux for the gth energy group at outer iteration level i and inner iteration level j be denoted by $\overline{\psi}_{\overline{j}g}^{(i,j)}$. These are defined by the corresponding modification of the inner iteration (26), (27), namely,

$$(\mathbf{I}_M - \mathbf{S}_g\hat{\mathbf{D}}_g)\overline{\psi}_{\overline{j}g}^{(i+1,j+1)} = \mathbf{S}_g\overline{\mathbf{D}}_g\overline{\psi}_{\overline{j}}^{(i+1,j)} + h_{\overline{j}g}^{(i+1)}, \tag{34}$$

where

$$h_{\overline{j}g}^{(i+1)} := \mathbf{S}_g\Big[\sum_{g'=1}^{g-1} \mathbf{L}_{gg'}\overline{\psi}_{\overline{j}g'}^{(i+1)} + \sum_{g'=g+1}^{G} \mathbf{U}_{gg'}\overline{\psi}_{\overline{j}g'}^{(i)}\Big] + \mathbf{S}_g q_g + b_g \tag{35}$$

and the starting values

$$\overline{\psi}_{\bar{j}g}^{(i+1,0)} = \overline{\psi}_{\bar{j}g}^{(i)} := \overline{\psi}_{\bar{j}g}^{(i,\bar{j})}. \tag{36}$$

The corresponding "best" approximation to the angular flux, over all groups, at outer iteration index i is $\overline{\psi}_{\bar{j}}^{(i)} \in \mathcal{C}^{\mathcal{G}}$, as defined by

$$\mathbf{P}_g \overline{\psi}_{\bar{j}}^{(i)} := \overline{\psi}_{\bar{j}g}^{(i)} = \overline{\psi}_{\bar{j}g}^{(i,\bar{j})}. \tag{37}$$

From (34) – (37) it is readily seen that $\overline{\psi}_{\bar{j}}^{(i)}$ determines $\overline{\psi}_{\bar{j}}^{(i+1)}$ via the iterative process

$$\overline{\psi}_{\bar{j}}^{(i+1)} = \mathbf{A}_{\bar{j}} \overline{\psi}_{\bar{j}}^{(i)} + \mathbf{B}_{\bar{j}}(\mathbf{S}q + b) + r_{\bar{j}}^{(i+1)}. \tag{38}$$

Here the linear operators $\mathbf{A}_{\bar{j}}$ and $\mathbf{B}_{\bar{j}}$, both mapping $\mathcal{C}^{\mathcal{G}}$ into itself, are defined inductively on g by

$$\begin{aligned} \mathbf{P}_g \mathbf{A}_{\bar{j}} f = &\sum_{j=0}^{\bar{j}-1} [(\mathbf{I}_M - \mathbf{S}_g \hat{\mathbf{D}}_g)^{-1} \mathbf{S}_g \overline{\mathbf{D}}_g]^j (\mathbf{I}_M - \mathbf{S}_g \hat{\mathbf{D}}_g)^{-1} \mathbf{S}_g \\ &\left[\sum_{g'=1}^{g-1} \mathbf{L}_{gg'} \mathbf{P}_{g'} \mathbf{A}_{\bar{j}} f + \sum_{g'=g+1}^{G} \mathbf{U}_{gg'} \mathbf{P}_{g'} f \right] \end{aligned} \tag{39}$$

and

$$\begin{aligned} \mathbf{P}_g \mathbf{B}_{\bar{j}} f = &\sum_{j=0}^{\bar{j}-1} [(\mathbf{I}_M - \mathbf{S}_g \hat{\mathbf{D}}_g)^{-1} \mathbf{S}_g \overline{\mathbf{D}}_g]^j \cdot (\mathbf{I}_M - \mathbf{S}_g \hat{\mathbf{D}}_g)^{-1} \\ &\left\{ \mathbf{S}_g \sum_{g'=1}^{g-1} \mathbf{L}_{gg'} \mathbf{P}_{g'} \mathbf{B}_{\bar{j}} f + \mathbf{P}_g f \right\}, \end{aligned} \tag{40}$$

for $f \in \mathcal{C}^{\mathcal{G}}$, and $r_{\bar{j}}^{(i+1)} \in \mathcal{C}^{\mathcal{G}}$ is defined by

$$\mathbf{P}_g r_{\bar{j}}^{(i)} = [(\mathbf{I}_M - \mathbf{S}_g \hat{\mathbf{D}}_g)^{-1} \mathbf{S}_g \overline{\mathbf{D}}_g]^{\bar{j}} \overline{\psi}_{\bar{j}g}^{(i,0)}. \tag{41}$$

The expectation is that $\overline{\psi}_{\overline{j}}^{(i)}$ will be a good approximation to $\psi^{(i)}$, where the latter are defined by the outer source iteration process (11). Thus we need to know that $\mathbf{A}_{\overline{j}}$ and $\mathbf{B}_{\overline{j}}$ respectively approximate $\mathbf{Q} := [\mathbf{I} - \mathbf{S}(\mathbf{D}+\mathbf{L})]^{-1}\mathbf{S}\mathbf{U}$ and $\mathbf{W} := [\mathbf{I} - \mathbf{S}(\mathbf{D}+\mathbf{L})]^{-1}$ and that the $r_{\overline{j}}^{(i)}$ are small. Now we begin a moderately lengthy sequence of technical details that are directed toward ultimately obtaining such results.

It is useful to introduce the operator $\hat{\mathbf{D}}$ and $\overline{\mathbf{D}}$, both mapping $\mathcal{C}^{\mathcal{G}}$ into itself, and respectively defined by

$$\mathbf{P}_g\hat{\mathbf{D}} = \hat{\mathbf{D}}_g\mathbf{P}_g, \ \mathbf{P}_g\overline{\mathbf{D}} := \overline{\mathbf{D}}_g\mathbf{P}_g,$$

where the $\hat{\mathbf{D}}_g$ and $\overline{\mathbf{D}}_g$ are as introduced in §3. The formulas given in the following proposition are easily established by direct computation and are useful tools in some of the calculations to follow.

PROPOSITION 5.1. *The following operator identities hold for* $g = 1, \ldots, G$:

$$\mathbf{P}_g\mathbf{L} = \sum_{g'=1}^{g-1} \mathbf{L}_{gg'}\mathbf{P}_{g'}, \tag{42}$$

$$\mathbf{P}_g\mathbf{D} = \mathbf{D}_g\mathbf{P}_g, \ \mathbf{P}_g\hat{\mathbf{D}} = \hat{\mathbf{D}}_g\mathbf{P}_g, \ \mathbf{P}_g\overline{\mathbf{D}} = \overline{\mathbf{D}}_g\mathbf{P}_g, \tag{43}$$

$$\mathbf{P}_g\mathbf{S} = \mathbf{S}_g\mathbf{P}_g, \tag{44}$$

$$\mathbf{P}_g(\mathbf{I} - \mathbf{S}\hat{\mathbf{D}})^{-1} = (\mathbf{I}_M - \mathbf{S}_g\hat{\mathbf{D}}_g)^{-1}\mathbf{P}_g. \tag{45}$$

LEMMA 5.2. *If* $\mathbf{W} := [\mathbf{I} - \mathbf{S}(\mathbf{D} + \mathbf{L})]^{-1}$, *then*

$$\begin{aligned} \mathbf{W} = \sum_{l=0}^{\infty} & \left\{ \sum_{j=0}^{\infty} [(\mathbf{I} - \mathbf{S}\hat{\mathbf{D}})^{-1}\mathbf{S}\overline{\mathbf{D}}]^j (\mathbf{I} - \mathbf{S}\hat{\mathbf{D}})^{-1}\mathbf{S}\mathbf{L} \right\}^l \\ & \cdot \left\{ \sum_{j=0}^{\infty} [(\mathbf{I} - \mathbf{S}\hat{\mathbf{D}})^{-1}\mathbf{S}\overline{\mathbf{D}}]^j \right\} (\mathbf{I} - \mathbf{S}\hat{\mathbf{D}})^{-1}, \end{aligned} \tag{46}$$

where the infinite series on the right all converge in the operator norm of $\mathcal{C}^{\mathcal{G}}$.

PROOF. Suppose $f = \mathbf{W}h$, where $h \in \mathcal{C}^{\mathcal{G}}$ is nonnegative. Then f also is nonnegative, by Corollary 2.6. Further, by comparison with the series in (16), the Neumann series $\sum_{n=0}^{\infty}(\mathbf{SD})^n$ converges, hence to $(\mathbf{I}-\mathbf{SD})^{-1}$, whence $(\mathbf{I}-\mathbf{SD})^{-1}$ also is positive. It follows that the partial sums

$$\sum_{l=0}^{n}[(\mathbf{I}-\mathbf{SD})^{-1}\mathbf{SL}](\mathbf{I}-\mathbf{SD})^{-1}h$$

are bounded above (by f). By the now familiar type of argument employed in the proof of Theorem 2.4, it follows that the corresponding series converges in $\mathcal{C}^{\mathcal{G}}$, and that its limit is f. This establishes

$$\mathbf{W} = \sum_{l=0}^{\infty}\{(\mathbf{I}-\mathbf{SD})^{-1}\mathbf{SL}\}^n(\mathbf{I}-\mathbf{SD})^{-1}, \tag{47}$$

with convergence in the strong sense, and uniform convergence follows from the equivalence of strong and uniform analyticity. (Theorem 3.10.1, Hille and Phillips [**11**].) But very similar arguments show that

$$(\mathbf{I}-\mathbf{SD})^{-1} = \sum_{j=0}^{\infty}[(\mathbf{I}-\mathbf{S}\hat{\mathbf{D}})^{-1}\mathbf{S}\overline{\mathbf{D}}]^j(\mathbf{I}-\mathbf{S}\hat{\mathbf{D}})^{-1},$$

and the desired equality (46) results from substituting this into (47). □

PROPOSITION 5.3. *If* $\mathbf{A}_{\bar{j}}, \mathbf{B}_{\bar{j}}$ *are as defined respectively by* (39) *and* (40), *then*

$$\begin{aligned}\mathbf{A}_{\bar{j}} = \sum_{l=0}^{\infty}\left\{\sum_{j=0}^{\bar{j}-1}[(\mathbf{I}-\mathbf{S}\hat{\mathbf{D}})^{-1}\mathbf{S}\overline{\mathbf{D}}]^j(\mathbf{I}-\mathbf{S}\hat{\mathbf{D}})^{-1}\mathbf{SL}\right\}^l \\ \cdot\left\{\sum_{j=0}^{\bar{j}}\left[\left(\mathbf{I}-\mathbf{S}\hat{\mathbf{D}}\right)^{-1}\mathbf{S}\overline{\mathbf{D}}\right]^j\right\}(\mathbf{I}-\mathbf{S}\hat{\mathbf{D}})^{-1}\mathbf{SU}\end{aligned} \tag{48}$$

and

$$\mathbf{B}_{\bar{j}} = \sum_{l=0}^{\infty}\left\{\sum_{j=0}^{\bar{j}-1}[(\mathbf{I}-\mathbf{S}\hat{\mathbf{D}})^{-1}\mathbf{S}\overline{\mathbf{D}}]^j(\mathbf{I}-\mathbf{S}\hat{\mathbf{D}})^{-1}\mathbf{S}\mathbf{L}\right\}^l \cdot\left\{\sum_{j=0}^{\bar{j}}[(\mathbf{I}-\mathbf{S}\hat{\mathbf{D}})^{-1}\mathbf{S}\overline{\mathbf{D}}]^j\right\}(\mathbf{I}-\mathbf{S}\hat{\mathbf{D}})^{-1}. \tag{49}$$

PROOF. By use of (42) – (45), equation (38) is seen to be simply the (group-) componentwise form of the equality

$$\mathbf{A}_{\bar{j}} = \sum_{j=0}^{\bar{j}-1}[(\mathbf{I}-\mathbf{S}\hat{\mathbf{D}})^{-1}\mathbf{S}\overline{\mathbf{D}}]^j(\mathbf{I}-\mathbf{S}\hat{\mathbf{D}})^{-1}\mathbf{S}(\mathbf{L}\mathbf{A}_{\bar{j}}+\mathbf{U}).$$

Equation (48), follows by solving this for $\mathbf{A}_{\bar{j}}$, as the series in (48) converges by comparison with that in (46). Equation (49) may be similarly obtained. □

If $\mathbf{A}$ and $\mathbf{B}$ are linear operators having as their common domain some linear space endowed with a cone and ranges contained in another (possibly the same) linear space so endowed, then we write $\mathbf{A} \geq \mathbf{B}$ if $\mathbf{A} - \mathbf{B}$ is a positive operator in the sense of mapping the cone in the domain space into the cone of the range space.

THEOREM 5.4. *Suppose* $\mathbf{B}_{\bar{j}}$ *is as defined by* (40). *Then*

$$\mathbf{B}_{\bar{j}} \leq \mathbf{W} := [\mathbf{I} - \mathbf{S}(\mathbf{D}+\mathbf{L})]^{-1} \tag{50}$$

for all natural numbers $\bar{j}$, *and, further,*

$$\lim_{\bar{j}\to\infty} \mathbf{B}_{\bar{j}} = \mathbf{W}, \tag{51}$$

where the convergence is relative to the operator norm on $C^{\mathcal{G}}$.

PROOF. The inequality (50) follows by termwise comparison of (46) and (40). As for (51), let $\varepsilon > 0$ be given, and choose a natural number

N such that the tail of the series in (47) is not greater than $\varepsilon/3$. By comparison, the corresponding tail of (45) is similarly bounded. If $\bar{j}$ then is picked sufficiently large so that each term from $l = 0$ to $l = N$ in (40) is within $\varepsilon/3N$ of the corresponding term in (46), then $\mathbf{B}_{\bar{j}}$ is seen to be within ε of $\mathbf{W}$. □

LEMMA 5.5. *Suppose the starting values* $\{\overline{\psi}_{\bar{j}g}^{(i,0)}\}$ *comprise a bounded subset of* $\mathcal{C}^M$, *uniformly in* $g = 1, \ldots, G$ *and all natural numbers* i *and* $\bar{j}$. *Then the sequences* $\left\{\overline{\psi}_{\bar{j}}^{(i)}\right\}_{i=0}^{\infty}$, *as defined by* (34) – (36) *and these starting values for the inner iterations, are bounded in* $\mathcal{C}^{\mathcal{G}}$, *uniformly in all sufficiently large* $\bar{j}$.

PROOF. From (38) we find

$$\overline{\psi}_{\bar{j}}^{(i+1)} = \sum_{l=0}^{i} (\mathbf{A}_{\bar{j}})^l [\mathbf{B}_{\bar{j}}(\mathbf{S}q + b) + r_{\bar{j}}^{(i+1-l)}], \tag{52}$$

where the $r_{\bar{j}}^{(l)}$ are given by (41). From Theorem 5.4 and (48), (49), we know that $\mathbf{A}_{\bar{j}} \to \mathbf{Q} = \mathbf{WSU}$ as $\bar{j} \to \infty$. As it follows from Theorem 2.7 that $r_\sigma(\mathbf{Q}) < 1$, there exists a natural number n and α satisfying $0 < \alpha < 1$ such that $\|\mathbf{Q}^n\| \le \alpha^n$. Therefore, $\|\mathbf{A}_{\bar{j}}^n\| \le \alpha^n$ for all sufficiently large $\bar{j}$, this same n, and a possibly different α satisfying the same conditions. From (52) then compute, for large $\bar{j}$,

$$\begin{aligned} \|\overline{\psi}_{\bar{j}}^{(i+1)}\| &\le \sum_{p=0}^{\infty} \Big\| \sum_{l=0}^{n-1} \mathbf{A}_{\bar{j}}^l \Big\| \cdot \|\mathbf{A}_{\bar{j}}^n\|^p (B\|\mathbf{S}q + b\| + \alpha) \\ &\le N\Big(\frac{1}{1-\alpha}\Big)(B\|\mathbf{S}q + b\| + \alpha). \end{aligned}$$

Here N is an upper bound, over all $\bar{j}$, for

$$\Big\| \sum_{l=0}^{n-1} \mathbf{A}_{\bar{j}}^l \Big\|,$$

B is a similar upper bound for $\|\mathbf{B}_{\bar{j}}\|$, and α is an upper bound for $r_{\bar{j}}^{(i)}$, over all natural numbers i and $\bar{j}$. These respective bounds exist, because $\mathbf{A}_{\bar{j}} \to \mathbf{Q}$, $\mathbf{B}_{\bar{j}} \to \mathbf{W}$ (both by virtue of Theorem 5.4), and $(\mathbf{I}_M - \mathbf{S}_g\hat{\mathbf{D}})^{-1}\mathbf{S}_g\overline{\mathbf{D}}_g$ has spectral radius less than unity (Theorem 3.3) and starting values uniformly bounded. □

REMARK 5.6. A somewhat shorter proof of Lemma 5.5 could be based upon the inequality (50); see the proof of Corollary 5.9 below for an illustration of this approach. However, we prefer also to illustrate the more direct approach used above in the proof of Lemma 5.5, as it might be useful in settings such that monotonicity arguments are unavailable.

THEOREM 5.7. *Suppose the starting values* $\{\overline{\psi}_{\bar{j}g}^{(i,0)}\}$ *are bounded in the sense of Lemma* 5.5. *Then the* $\{\overline{\psi}_{\bar{j}g}^{(i)}\}$, *as defined by* (34) – (36) *and these starting values for the inner iterations along with an arbitrary starting value in* $C^{\mathcal{G}}$ *for the outer iteration, approximate the exact angular flux* ψ, *as defined by* (4) *through* (6), *in the following sense: Given any* $\varepsilon > 0$, *there exist natural numbers* I_0 *and* J_0 *such that if* $i \geq I_0$ *and* $\bar{j} \geq J_0$, *then* $\|\overline{\psi}_{\bar{j}}^{(i)} - \psi\| \leq \varepsilon$ *(where the norm is that of* $C^{\mathcal{G}}$*).*

PROOF. Let $u_{\bar{j}}^{(i)} := \overline{\psi}_{\bar{j}}^{(i)} - \psi^{(i)}$, where the $\psi^{(i)}$ are the approximate angular fluxes as defined by the outer source iteration. By virtue of Corollary 2.8, it suffices to show that

$$\lim_{i\to\infty} u_{\bar{j}}^{(i)} = 0,$$

uniformly in all sufficiently large $\bar{j}$. From (11) and (38) we find

$$u_{\bar{j}}^{(i+1)} = \mathbf{Q}u_{\bar{j}}^{(i)} + w_{\bar{j}}^{(i+1)},$$

where

$$w_{\bar{j}}^{(i+1)} = (\mathbf{A}_{\bar{j}} - \mathbf{Q})\overline{\psi}_{\bar{j}}^{(i)} + (\mathbf{B}_{\bar{j}} - \mathbf{W})(\mathbf{S}q + b) + r_{\bar{j}}^{(i+1)}$$

and the $r_{\bar{j}}^{(i+1)}$ are defined by (41). It follows that

$$u_{\bar{j}}^{(i+1)} = \sum_{i'=0}^{i} \mathbf{Q}^{i'} w_{\bar{j}}^{(i+1-i')} + \mathbf{Q}^{i+1}u_{\bar{j}}^{(0)}.$$

Now $\mathbf{Q}$ has spectral radius less than one (Corollary 2.8), and the $w_{\bar{j}}^{(i+1)}$ are bounded in both $\bar{j}$ and i (Theorem 5.4, Lemma 5.5, Theorem 3.3 and uniform boundedness of the starting values for the inner iterations), whence there exists I_0 such that

$$\sum_{i'=I_0+1}^{i} \mathbf{Q}^{i'} w_{\bar{j}}^{(i+1-i')} + \mathbf{Q}^{i+1} u_{\bar{j}}^{(0)}$$

is bounded by $\varepsilon/2$ if $i \geq I_0$. Again, by Theorem 5.4, Lemma 5.5, Theorem 3.3 and uniform boundedness of the starting values for the inner iterations, there exists J_0 such that if $\bar{j} \geq J_0$, then

$$\sum_{i'=0}^{I_0} \mathbf{Q}^{i'} w_{\bar{j}}^{(i+1-i')}$$

is bounded by $\varepsilon/2$. □

Now extend the previous considerations of this section to the situation that the inner iterations are terminated at a step possibly depending on the particular energy group and outer iteration index. Specifically, let $\mathcal{N}$ and $\mathcal{N}_G$ denote respectively the natural numbers and the first G natural numbers. Suppose that the inner iteration associated with the ith outer iteration index and group g is terminated after step $j = J(i,g)$, where $J : \mathcal{N} \times \mathcal{N}_G \to \mathcal{N}$ is a *stopping sequence.* Given such a stopping sequence, set

$$m_0(J) = \min\{J(i,g) : (i,g) \in \mathcal{N} \times \mathcal{N}_G\} \tag{53}$$

and denote the jth inner approximation to the angular flux at group g and outer interation index i by $\psi_{Jg}^{(i,j)}$. The corresponding modification of the inner iteration (26), (27) is

$$(\mathbf{I}_M - \mathbf{S}_g\hat{\mathbf{D}}_g)\psi_{Jg}^{(i+1,j+1)} = \mathbf{S}_g\overline{\mathbf{D}}_g\psi_{Jg}^{(i+1,j)} + h_{Jg}^{(i+1)}, \tag{54}$$

where

$$h_{Jg}^{(i+1)} := \mathbf{S}_g\left[\sum_{g'=1}^{g-1} \mathbf{L}_{gg'}\tilde{\psi}_{Jg'}^{(i+1)} + \sum_{g'=g+1}^{G} \mathbf{U}_{gg'}\tilde{\psi}_{Jg'}^{(i)}\right] + \mathbf{S}_g q_g + b_g \tag{55}$$

and

$$\tilde{\psi}_{Jg}^{(i)} := \psi_{Jg}^{(i,J(i,g))}. \tag{56}$$

The corresponding "best" approximation to the angular flux at outer iteration index i is $\tilde{\psi}_J^{(i)} \in \mathcal{C}^{\mathcal{G}}$, as defined by

$$\mathbf{P}_g \tilde{\psi}_J^{(i)} := \tilde{\psi}_{Jg}^{(i,J(i,g))}. \tag{57}$$

From (54) – (57) the relation between $\tilde{\psi}_J^{(i)}$ and $\tilde{\psi}_J^{(i+1)}$ can be written as the nonstationary iterative process

$$\tilde{\psi}_J^{(i+1)} = \tilde{\mathbf{A}}_J^{(i+1)} \tilde{\psi}_J^{(i)} + \tilde{\mathbf{B}}_J^{(i+1)} (\mathbf{S}q + b) + r_J^{(i+1)}, \tag{58}$$

where $\tilde{\mathbf{A}}_J^{(i)}, \tilde{\mathbf{B}}_J^{(i)}$ and $r_J^{(i)}$ are defined respectively by (39) – (41), except with $\overline{j}$ replaced by $J(i,g)$. As before, we need to establish that each $\mathbf{A}_J^{(i)}$ and $\mathbf{B}_J^{(i)}$, respectively, approximate $\mathbf{Q}$ and $\mathbf{W}$ and that $r_J^{(i+1)} \to 0$, with large i and $m_0(J)$. The crucial result for these is

LEMMA 5.8. *If J is a stopping sequence with $m_0 = m_0(J)$, then, for each natural number i, we have*

$$\mathbf{B}_{m_0} \leq \tilde{\mathbf{B}}_J^{(i)} \leq \mathbf{W}, \tag{59}$$

whence $\tilde{\mathbf{B}}_J^{(i)} \to \mathbf{W}$ in the operator norm of $C^{\mathcal{G}}$, uniformly in all natural numbers i, as $m_0(J) \to \infty$.

PROOF. The first inequality in (59) follows by induction based upon a termwise comparison of (40) and the corresponding defining expression for $\tilde{\mathbf{B}}_J^{(i)}$. A similar comparison of the latter with the action of each $\mathbf{P}_g$ upon the readily established equality

$$\mathbf{W} = \sum_{j=0}^{\infty} [(\mathbf{I} - \mathbf{S}\hat{\mathbf{D}})^{-1} \mathbf{S}\overline{\mathbf{D}}]^j (\mathbf{I} - \mathbf{S}\hat{\mathbf{D}})^{-1} (\mathbf{I} + \mathbf{SLW})$$

similarly establishes the second inequality of (59). The asserted convergence follows directly from (59), which completes our outline of the proof of Lemma 5.8. □

COROLLARY 5.9. *If the assumptions of Lemma* 5.5 *are satisfied, then the sequences* $\{\tilde{\psi}_J^{(i)}\}_{i=0}^{\infty}$, *as defined by* (54) *through* (57) *and the starting values for the inner iterations, are bounded uniformly in all stopping sequences* J.

PROOF. From (58) and Lemma 5.7 we have

$$|\tilde{\psi}_J^{(i+1)}| \leq \mathbf{Q}|\tilde{\psi}_J^{(i)}| + \mathbf{W}(\mathbf{S}q + b) + |r_J^{(i)}|,$$

where

$$|\tilde{\psi}_J^{(i+1)}| \leq \sum_{i'=1}^{i} \mathbf{Q}^{i'}[\mathbf{W}(\mathbf{S}q + b) + |r_J^{(i-i')}|].$$

But $\mathbf{Q}$ has spectral radius less than unity, and the $r_J^{(i)}$ are uniformly bounded as in the proof of Lemma 5.5, which yields the desired result. □

THEOREM 5.10. *Suppose the starting values* $\{\tilde{\psi}_{Jg}^{(i,0)}\}$ *are bounded in the sense of Lemma* 5.5. *Then the* $\{\tilde{\psi}_J^{(i)}\}$, *as defined by* (54) – (56) *along with these starting values for the inner iterations and an arbitrary starting value in* $C^{\mathcal{G}}$ *for the outer iteration, approximate the exact angular flux, as determined by* (4) – (6), *in the following sense: Given any* $\varepsilon > 0$, *there exist natural numbers* I_0 *and* M_0, *such that if* $i \geq I_0$ *and* J *is a stopping sequence with* $m_0(J) \geq M_0$, *then* $\|\tilde{\psi}_J^{(i)} - \psi\| \leq \varepsilon$ *(where the norm is that of* $C^{\mathcal{G}}$*).*

PROOF. Let $u_J^{(i)} := \tilde{\psi}_J^{(i)} - \psi^{(i)}$. As in the proof of Theorem 5.6, it suffices to show that

$$\lim_{i\to\infty} u_J^{(i)} = 0,$$

uniformly in all stopping sequences having sufficiently large values of m_0. From (11) and (58), we find

$$u_J^{(i+1)} = \mathbf{Q}u_J^{(i)} + w_J^{(i+1)},$$

where

$$w_J^{(i+1)} = (\mathbf{A}_J^{(i+1)} - \mathbf{Q})\tilde{\psi}_j^{(i)} + (\mathbf{B}_j - \mathbf{W})(\mathbf{S}q + b) + r_J^{(i+1)}.$$

The remainder of the proof is essentially identical to that of Theorem 5.7, except with Theorem 5.4 and Lemma 5.5 replaced, respectively, by Lemma 5.8 and Corollary 5.9. This completes both the proof of Theorem 5.10 and the technical portion of this paper. □

6. Concluding remarks. Brickner, Hiromoto, and Wienke [**16-18**] have reported computational experiments on a variety of parallel implementations of source iteration. The present work originated from the desire to analyze and better understand these parallel versions; in order to provide a basis for this, we found it necessary to further study the classical several implementation of source iteration.

In practice most implementations of source iteration in computer codes permit the user to control the number or accuracy of the inner iterations, but not in a manner that depends upon the current accuracy in the outer iteration. (See [**15, 19**] for computational experiments on the combined effect of these iterations.) However, one expects that an optimal strategy would permit such dependence. We expect it to be possible to determine appropriate such strategies by further pursuing the type of analysis presented herein; Golub and Overton [**8**] recently presented such results in a finite-dimensional setting.

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