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SOLUTION OF RADIATIVE TRANSFER PROBLEMS USING THE INVARIANT S_n METHOD

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Summary

The discrete ordinate difference equations of radiative transfer for a slab in the form presented by Carlson and by Lathrop & Carlson can be written in a form consistent with principles of invariance. It is shown that this permits solution of the equations, without the need for iteration in scattering problems, by a method which converges in the limit to that of Rybicki & Usher. The new method is economical to use, both in respect of storage and of computing time, and may be preferable to that of Rybicki & Usher in problems with anisotropic phase functions.

The mathematical structure of the equations and its implications are briefly discussed. Specimen numerical results are provided for diffuse reflection from an isotropically scattering homogeneous slab and compared with results published by other investigators.

1. *Introduction.* Many different methods have been proposed for the numerical solution of the equation of radiative transfer. These methods involve discretization of the angle variables and possibly of space variables as well. One of the best known of these techniques is the method of discrete ordinates as described, for example, in Chandrasekhar's monograph (1950). In that work, the discretization was applied only to the angle variables, from which, in the case of a plane-parallel atmosphere, a system of simultaneous ordinary differential equations could be obtained. These differential equations could be solved by classical methods to obtain an approximate solution. One disadvantage of this analytical work is that it cannot be easily generalized to treat non-uniform media. More difficulties arise when one tries to treat problems in curvilinear coordinate systems.

A numerical version of the discrete ordinates technique which has been much used in reactor neutronics calculations is that of B. G. Carlson and his collaborators. A survey of this work is given for example by Carlson (1963) and Lathrop & Carlson (1967). The differential operator of radiative transfer can be written as a divergence and so, by integrating the radiative transfer equation over a small but finite volume in the space of the independent variables and making use of a mean value theorem for integrals, one can construct difference equations that clearly conserve flux. These difference equations can be formulated for quite general non-uniform media and for arbitrary curvilinear coordinate systems. They can be solved in a stable manner, by a method which requires an iterative procedure whenever the medium both scatters and absorbs radiation. This iteration converges satisfactorily if the optical thickness of the medium is not too high and the albedo for single scattering is not too close to unity. Otherwise the iteration may converge very slowly and it is hard to obtain a good solution.

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Invariance methods have not usually been considered in this context, which is somewhat surprising since they are only the expression of a conservation relation for finite partitioning of a physical system. Most discussions of principles of invariance (e.g. Chandrasekhar 1950; Mullikin 1964) lead to a system of non-linear integro-differential equations on which attention is subsequently focused. In the words used by Preisendorfer (1965), principles of invariance are ' apparently abiogenetic '. Preisendorfer goes on to show that this is not so, and that the principles of invariance are a natural property of the reflection and transmission operators associated with subdivisions of the region of interest. Since Carlson's difference equations are known to be conservative, we might expect to see invariance principles deduced from them in the way that Preisendorfer has suggested. This conjecture was one of the sources of inspiration for the work described in this paper.

With any numerical method, it is important to know what discretization errors can be tolerated in order to obtain a result with specified minimum accuracy. Hitherto, the numerical analysis of Carlson's difference equations has hardly progressed beyond a qualitative demonstration of stability. This has largely been because of the complexity of their structure. We have sought to overcome this by rewriting the equations in what we call ' invariant S_n ' form. The method of doing this is set out in Section 2 for the case of a plane-parallel slab. The result can be expressed in matrix form and the non-zero submatrices can be interpreted as approximations to reflection and transmission operators for the elementary slab zones into which the system has been decomposed. The structure of the matrix facilitates the desired analysis and enables us to construct a simple direct method of solution that turns out to converge, in the limit of vanishingly small zone thickness, to the equations recently put forward by Rybicki & Usher (1966). In this way we need no longer iterate the solution for scattering problems.

The full analysis of our method is too lengthy to produce in a single paper, and we have therefore contented ourselves with a sketch of the results obtained, and a brief account of a solution for a simple problem.

2. *The DSN equations of Carlson for a slab.* We describe first the basic difference equations that we are to examine. A full derivation in the general case is given by Carlson (1963) and Lathrop & Carlson (1967) and we refer the reader to those papers for details. We wish to find an approximate solution for the specific intensity $I(x, \mu)$ at depth x travelling in a direction making an angle whose cosine is μ with the normal in the positive x-direction, where, for $0 < \mu \leqslant 1$, $0 < x < x_{N+1}$,

$$\left[\mu \frac{\partial}{\partial x} + \sigma(x)\right] I(x, \mu) = \sigma(x)\left\{[1 - \omega(x)]B(x) + \tfrac{1}{2}\omega(x) \int_{-1}^{+1} p(x, \mu, \mu')I(x, \mu')\, d\mu'\right\},$$

$$\left[-\mu \frac{\partial}{\partial x} + \sigma(x)\right] I(x, \mu) = \sigma(x)\left\{[1 - \omega(x)]B(x) + \tfrac{1}{2}\omega(x) \int_{-1}^{+1} p(x, -\mu, \mu')I(x, \mu')\, d\mu'\right\}, \quad (2.1)$$

for intensities in the positive and negative x-direction respectively. (This is not the usual convention in astrophysical work, but it is less confusing to have positive directed intensities in the same sense as x increases.) The functions $\sigma(x)$, $\omega(x)$, $B(x)$ and $p(x, \mu, \mu')$ are prescribed (in general, piecewise continuous) functions of their

arguments, subject to the conditions

$$B(x) \geqslant 0, \quad \sigma(x) \geqslant 0, \quad 0 \leqslant \omega(x) \leqslant 1, \quad 0 < x < x_{N+1} \tag{2.2}$$

and

$$\tfrac{1}{2}\int_{-1}^{+1} p(x, \mu, \mu')\, d\mu' = 1, \quad \begin{cases} -1 \leqslant \mu \leqslant 1 \\ 0 < x < x_{N+1} \end{cases} \qquad p(x, \mu, \mu') \geqslant 0. \tag{2.3}$$

Together with equation (2.1) and the functions just described, we require boundary values $I(0, \mu)$, $I(x_{N+1}, -\mu)$, $0 < \mu \leqslant 1$ to complete the specification of our problem.

By using the procedure outlined in Section 1, and fully described in the references cited above, we replace equations (2.1) by a system of difference equations. We divide the region $0 = x_1 < x < x_{N+1}$ into N cells or layers by planes $x = x_i$, $i = 2,3,\ldots, N$, where $x_i \leqslant x_j$ whenever $i \leqslant j$. We also choose m discrete directions $0 \leqslant \mu_1 \leqslant \ldots \leqslant \mu_m \leqslant 1$ with which we associate quadrature weights $c_1, \ldots, c_m$. At each plane we can define column vectors

$$u_n^+ = \begin{bmatrix} u_{n,1} \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ u_{n,m} \end{bmatrix}, \quad u_n^- = \begin{bmatrix} u_{n,-1} \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ u_{n,-m} \end{bmatrix}, \quad n = 1,2,\ldots, N+1, \tag{2.4}$$

where

$$u_{n,j} = I(x_n, \mu_j), \quad u_{n,-j} = I(x_n, -\mu_j). \tag{2.5}$$

From now on, we shall not need to refer to intensities by the symbol I, and we shall reserve I for the unit matrix of appropriate order in the remainder of the paper. If M denotes the diagonal matrix

$$M = [\mu_i \delta_{ij}] \tag{2.6}$$

and c the corresponding matrix of quadrature weights, the total flux in positive directions is defined by

$$\pi F_n^+ = 2\pi \|Mcu_n^+\| = 2\pi \|u_n^+\|_F, \tag{2.7}$$

where the expression $\|u\|$ is the vector norm defined by

$$\|u\| = \sum_{j=1}^{m} |u_j|. \tag{2.8}$$

The net flux in the positive direction is given by

$$\pi F_n = \pi(F_n^+ - F_n^-) \tag{2.9}$$

in the usual way. The modified norm $\|\ldots\|_F$ requires premultiplication of the vector by the matrix $cM = Mc$ before using equation (2.8). This operation is the discrete equivalent of multiplication by μ and integration over $0 < \mu \leqslant 1$. In terms of this matrix notation, the difference equations replacing equation (2.1) become

$$-Mu_n^+ + Mu_{n+1}^+ + \tau_{n+1/2} u_{n+1/2}^+ = \tau_{n+1/2}\{(1 - \omega_{n+1/2}) b_{n+1/2} + \tfrac{1}{2}\omega_{n+1/2}[p_{n+1/2}^{++} cu_{n+1/2}^+ + p_{n+1/2}^{+-} cu_{n+1/2}^-]\}, \tag{2.10}$$

$$-Mu_{n+1}^- + Mu_n^- + \tau_{n+1/2} u_{n+1/2}^- = \tau_{n+1/2}\{(1 - \omega_{n+1/2}) b_{n+1/2} + \tfrac{1}{2}\omega_{n+1/2}[p_{n+1/2}^{-+} cu_{n+1/2}^+ + p_{n+1/2}^{--} cu_{n+1/2}^-]\},$$

for each layer $x_n < x < x_{u+1}$, $n = 1,2,\ldots,N$. Subscripts n, $n+1$ associate vectors with the bounding planes x_n, x_{n+1}. Subscripts $n+\frac{1}{2}$ associate quantities (scalar or vector) with cell averages. For example, we write

$$\tau_{n+1/2} = \int_{x_n}^{x_{n+1}} \sigma(x)\,dx = \sigma_{n+1/2}(x_{n+1}-x_n) \tag{2.11}$$

defining $\sigma_{n+1/2}$. On the right hand side of equation (2.10), $b_{n+1/2}$ is a vector with m components each equal to some mean value of $B(x)$ for the cell. The matrices $p_{n+1/2}{}^{++}$, $p_{n+1/2}{}^{+-}$, etc. of order $m \times m$, are symmetric and we have

$$p_{n+1/2}{}^{++} = p_{n+1/2}{}^{--}, \quad p_{n+1/2}{}^{+-} = p_{n+1/2}{}^{-+}, \tag{2.12}$$

where

$$\left.\begin{aligned} p(x, \mu_i, \mu_j) &= p_{n+1/2}{}^{++}, \\ p(x, \mu_i, -\mu_j) &= p_{n+1/2}{}^{+-}, \\ p(x, -\mu_i, \mu_j) &= p_{n+1/2}{}^{-+}, \\ p(x, -\mu_i, -\mu_j) &= p_{n+1/2}{}^{--}, \end{aligned}\right\} \quad \begin{matrix} 0 < \mu_i \leqslant 1 \\ 0 < \mu_j \leqslant 1 \end{matrix}$$

for some x in $x_n < x < x_{n+1/2}$. As we have said, matrix products with a factor c imply integration over μ; thus, if $\mu > 0$,

$$p_{n+1/2}{}^{+-} c u_{n+1/2}{}^{-} \approx \int_0^1 p(x, \mu, -\mu') I(x, -\mu')\,d\mu'. \tag{2.13}$$

The normalizing condition (2.3) may be written

$$\tfrac{1}{2} \sum_{j=1}^{m} (p_{ij}{}^{++} + p_{ij}{}^{+-}) c_j = 1, \quad 1 \leqslant i \leqslant m \tag{2.14}$$

or, since the matrices are symmetric and equation (2.12) holds

$$\tfrac{1}{2} \sum_{i=1}^{m} c_i (p_{ij}{}^{++} + p_{ij}{}^{-+}) = 1, \quad 1 \leqslant j \leqslant m. \tag{2.15}$$

The last relation shows that

$$\|\tfrac{1}{2} c(p^{++} + p^{-+})\| = 1, \tag{2.16}$$

where the matrix norm used here is subordinate to the vector norm (2.8), namely

$$\|A\| = \max_j \sum_{i=1}^{m} |A_{ij}|, \tag{2.17}$$

(Varga 1962, p. 15). A second relation can be obtained by interchanging plus and minus signs in the superscripts of equations (2.15) and (2.16).

If we consider equations (2.10) together with boundary conditions giving $u_1{}^{+}$, $u_{N+1}{}^{-}$, we see that we have too many unknowns. We need auxiliary equations to express $u_{n+1/2}{}^{+}$, $u_{n+1/2}{}^{-}$ in terms of the remaining vectors to resolve the difficulty. These auxiliary equations must embody some assumption about the physical shape of the radiation field in a cell. This is, of course, unknown. We therefore suppose that $u_{n+1/2}{}^{+}$, $u_{n+1/2}{}^{-}$ may be expressed as a weighted mean of the interface intensities

$$\begin{aligned} (I - X_{n+1/2}{}^{+}) u_n{}^{+} + X_{n+1/2}{}^{+} u_{n+1}{}^{+} &= u_{n+1/2}{}^{+}, \\ (I - X_{n+1/2}{}^{-}) u_{n+1}{}^{-} + X_{n+1/2}{}^{-} u_n{}^{-} &= u_{n+1/2}{}^{-}, \end{aligned} \tag{2.18}$$

where the $X_{n+1/2}$ are diagonal $m \times m$ matrices. Standard choices (Carlson 1963) are $X_{n+1/2} = \frac{1}{2}I$ (' diamond ' scheme) and $X_{n+1/2} = I$ (' step ' scheme). Other choices of an intermediate character are possible (Grant 1968).

Methods of solving the complete system of equations (2.10) and (2.18) are described in the papers by Lathrop & Carlson already cited. The solution is explicit if scattering is absent; otherwise it is necessary to iterate. These methods do not lend themselves to mathematical analysis. We shall describe a transformation of the equations which eliminates the need to iterate for a scattering medium and allows us to obtain a greater understanding of the structure of our approximations.

3. *The invariant DSN equations.* In order to exhibit the structure of the equations we need to consider each cell independently as a slab in its own right and to exhibit the dependence of its radiation field on the sources incident from neighbouring cells in the slab. Since, for example, u_n^+ refers to the common interface of two cells, it will appear in the equations for both. In order to separate these equations we need to define vectors $U_{n+1/2}$ associated with each cell alone. These vectors have dimension $6m$ and may be partitioned in the form

$$U_{n+1/2} = \begin{bmatrix} \mathbf{U}_{n+1/2^+} \\ \\ \mathbf{U}_{n+1/2^-} \end{bmatrix}, \quad \mathbf{U}_{n+1/2^+} = \begin{bmatrix} u_n^+ \\ u_{n+1}^+ \\ u_{n+1/2}^+ \end{bmatrix}, \quad \mathbf{U}_{n+1/2^-} = \begin{bmatrix} u_{n+1}^- \\ u_n^- \\ u_{n+1/2}^- \end{bmatrix},$$

$$n = 1,2,\ldots,N \quad (3.1)$$

This structure has been chosen so that for each vector the first m rows refer to input, the next m rows to output, and the last m rows to central intensities in either direction. The continuity of flux at an interface is expressed by the identity

$$\begin{bmatrix} I & . & . \\ . & . & . \\ . & . & . \end{bmatrix} \mathbf{U}_{n+1/2^+} = \begin{bmatrix} . & I & . \\ . & . & . \\ . & . & . \end{bmatrix} \mathbf{U}_{n-1/2^+}, \quad n = 1,\ldots,N \qquad (3.2)$$

or

$$\begin{bmatrix} I & . & . \\ . & . & . \\ . & . & . \end{bmatrix} \mathbf{U}_{n+1/2^-} = \begin{bmatrix} . & I & . \\ . & . & . \\ . & . & . \end{bmatrix} \mathbf{U}_{n+3/2^-}, \quad n = 1,\ldots,N. \qquad (3.3)$$

These identities involve the fluxes incident on the boundary for $n = 1$ in the case of equation (3.2) and $n = N$ in the case of equation (3.3). It is convenient to include such fluxes by introducing fictitious cells associated with suffices $\frac{1}{2}$ and $N+\frac{3}{2}$ for which

$$\mathbf{U}_{1/2^+} = \begin{bmatrix} . \\ u_1^+ \\ . \end{bmatrix}, \quad \mathbf{U}_{N+3/2^-} = \begin{bmatrix} . \\ u_{N+1}^- \\ . \end{bmatrix} \qquad (3.4)$$

are prescribed. (The corresponding vectors $\mathbf{U}_{1/2^-}$ and $\mathbf{U}_{N+3/2^+}$ are irrelevant.) We now write equations (2.10) and (2.18) in terms of the vectors $\mathbf{U}_{n+1/2^+}$, $\mathbf{U}_{n+1/2^-}$ and

combine the equations with equations (3.2) and (3.3). The result is

$$\begin{bmatrix} I & . & . \\ I-X_{n+1/2}{}^{+} & X_{n+1/2}{}^{+} & -I \\ -M & M & \tau_{n+1/2}[I-\frac{1}{2}\omega_{n+1/2}\mathfrak{p}_{n+1/2}{}^{++}c] \end{bmatrix} \mathbf{U}_{n+1/2}{}^{+}$$

$$-\begin{bmatrix} . & . & . \\ . & . & . \\ . & . & \frac{1}{2}\tau_{n+1/2}\omega_{n+1/2}\mathfrak{p}_{n+1/2}{}^{+-}c \end{bmatrix} \mathbf{U}_{n+1/2}{}^{-}$$

$$=\begin{bmatrix} . & I & . \\ . & . & . \\ . & . & . \end{bmatrix} \mathbf{U}_{n-1/2}{}^{+}+\tau_{n+1/2}(1-\omega_{n+1/2})\begin{bmatrix} . \\ . \\ b_{n+1/2} \end{bmatrix}, \quad n = 1,2,\ldots,N \tag{3.5}$$

for the plus direction. The corresponding equation for the minus direction has the same matrix structure, plus and minus being interchanged, whilst the first term on the right hand side contains $\mathbf{U}_{n+3/2}{}^{-}$.

Assuming, for the moment, that the necessary matrix inverses exist, straightforward but tedious manipulation, which has been relegated to the Appendix, shows that the cell vector $U_{n+1/2}$ satisfies the equation

$$-A_{n+1/2}U_{n-1/2}+U_{n+1/2}-B_{n+1/2}U_{n+3/2} = \Sigma_{n+1/2}, \tag{3.6}$$

for $n = 1,2,\ldots,N$. The matrices $A_{n+1/2}$, $B_{n+1/2}$ only couple the relevant intensities incident on the cell boundary to $U_{n+1/2}$. This can be seen by examining their block structure; in terms of $3m\times 3m$ blocks we may write

$$A_{n+1/2} = \begin{bmatrix} \mathbf{T}(n+1,n) & . \\ \mathbf{R}(n+1,n) & . \end{bmatrix}, \quad B_{n+1/2} = \begin{bmatrix} . & \mathbf{R}(n,n+1) \\ . & \mathbf{T}(n,n+1) \end{bmatrix}. \tag{3.7}$$

The corresponding partition of the source vector $\Sigma_{n+1/2}$ is written

$$\Sigma_{n+1/2} = \begin{bmatrix} \mathbf{\Sigma}_{n+1/2}{}^{+} \\ \mathbf{\Sigma}_{n+1/2}{}^{-} \end{bmatrix}$$

as in equation (A.9).

Each block $\mathbf{T}$ or $\mathbf{R}$ can itself be partitioned into $m\times m$ blocks so that

$$\mathbf{T}(i,j) = \begin{bmatrix} . & I & . \\ . & T(i,j) & . \\ . & T_c(i,j) & . \end{bmatrix}, \quad \mathbf{R}(i,j) = \begin{bmatrix} . & . & . \\ . & R(i,j) & . \\ . & R_c(i,j) & . \end{bmatrix}. \tag{3.8}$$

Thus $A_{n+1/2}$ only couples the vector $u_n{}^{+}$ and $B_{n+1/2}$ couples the vector $u_{n+1}{}^{-}$ as required.

If we write out the equations in detail, we find, for example

$$-\mathbf{T}(n+1,n)\mathbf{U}_{n+1/2-}-\mathbf{R}(n,n+1)\mathbf{U}_{n+3/2}{}^{-} = \mathbf{\Sigma}_{n+1/2}{}^{+}, \tag{3.9}$$

which is equivalent to the three equations

$$\begin{aligned} -u_n{}^{+}+u_n{}^{+} &= 0, \\ -T(n+1,n)u_n{}^{+}+u_{n+1}{}^{+}-R(n,n+1)u_{n+1}{}^{-} &= \Sigma_{n+1/2}{}^{+}, \\ -T_c(n+1,n)u_n{}^{+}+u_{n+1/2}{}^{+}-R_c(n,n+1)u_{n+1}{}^{-} &= \Sigma_{c,n+1/2}{}^{+}. \end{aligned} \tag{3.10}$$

The first of these equations expresses the continuity of flux as in equation (3.1). The

last equation shows that $u_{n+1/2}$ can be simply written in terms of the incident fluxes on the boundary. It is clear that we can in fact dispense with this equation for the purposes of computation and deal only with the boundary fluxes. The auxiliary equations (2.18) can then be invoked to obtain the omitted central intensity vectors if they are needed.

In this case, equations (3.6) remain valid but the vectors $U_{n+1/2}$, $\mathbf{U}_{n+1/2}{}^{+}$, $\mathbf{U}_{n+1/2}{}^{-}$ must now be interpreted as of dimension $4m$, $2m$, $2m$ respectively, since

$$\mathbf{U}_{n+1/2}{}^{+} = \begin{bmatrix} u_n{}^{+} \\ u_{n+1}{}^{+} \end{bmatrix}, \quad \mathbf{U}_{n+1/2}{}^{-} = \begin{bmatrix} u_{n+1}{}^{-} \\ u_n{}^{-} \end{bmatrix} \tag{3.11}$$

are both of dimension $2m$. We shall use the same notation for the truncated vectors and operators for the sake of economy, as no confusion is likely to arise. Again equation (3.7) will be valid with the interpretation

$$\mathbf{T}(i,j) = \begin{bmatrix} \cdot & I \\ \cdot & T(i,j) \end{bmatrix}, \quad \mathbf{R}(i,j) = \begin{bmatrix} \cdot & \cdot \\ \cdot & R(i,j) \end{bmatrix}, \quad j = i \pm 1. \tag{3.12}$$

Finally

$$\mathbf{\Sigma}_{n+1/2}{}^{+} = \begin{bmatrix} \cdot \\ \Sigma_{n+1/2}{}^{+} \end{bmatrix}, \quad \mathbf{\Sigma}_{n+1/2}{}^{-} = \begin{bmatrix} \cdot \\ \Sigma_{n+1/2}{}^{-} \end{bmatrix}. \tag{3.13}$$

4. *Solution of the invariant DSN equations.* The system (3.6) can be solved in a particularly rapid and economical fashion by exploiting its block tridiagonal structure. Assuming for the present that all the required inverses exist, we define a set of $4m \times 4m$ matrices $C_{n+1/2}$, $D_{n+1/2}$ and $E_{n+1/2}$, $n = 1,2,\ldots,N$ using the recursive system

$$\begin{aligned} C_{1/2} &= 0, \\ D_{n+1/2} &= [I - A_{n+1/2}C_{n-1/2}]^{-1}, \\ C_{n+1/2} &= D_{n+1/2}B_{n+1/2}, \\ E_{n+1/2} &= D_{n+1/2}A_{n+1/2}. \end{aligned} \tag{4.1}$$

We also define vectors $V_{n+1/2}$, of dimension $4m$, by way of the system

$$\begin{aligned} V_{1/2} &= U_{1/2} = \begin{bmatrix} \mathbf{U}_{1/2}{}^{+} \\ \cdot \end{bmatrix}, \\ V_{n+1/2} &= E_{n+1/2}V_{n-1/2} + D_{n+1/2}\Sigma_{n+1/2}, \end{aligned} \tag{4.2}$$

for $n = 1,2,\ldots,N$, where $\mathbf{U}_{1/2}{}^{+}$ denotes the $2m$-dimensional form of the first of equations (3.4). Then the solutions $U_{n+1/2}$ can be computed from the system

$$\begin{aligned} U_{N+3/2} &= \begin{bmatrix} \cdot \\ \mathbf{U}_{N+3/2}{}^{-} \end{bmatrix}, \\ U_{n+1/2} &= C_{n+1/2}U_{n+3/2} + V_{n+1/2}, \end{aligned} \tag{4.3}$$

for $n = N, N-1,\ldots,1$ in succession. Here $\mathbf{U}_{N+3/2}{}^{-}$ is defined by the $2m$-dimensional form of the second of equations (3.4).

For the most economical implementation of these equations, it is worthwhile to decompose them into m-dimensional form, thus making best use of the sparseness of the matrices. At the same time one obtains much physical insight by so doing. We shall use heavy type to denote $2m \times 2m$ blocks into which the C, D, and E matrices can be decomposed. These $2m \times 2m$ blocks will themselves be decomposed

into $m \times m$ blocks, which will appear in light type. Thus it is easy to verify the decomposition

$$C_{n+1/2} = \begin{bmatrix} . & \mathbf{R}(1, n+1) \\ . & \hat{\mathbf{T}}(n, n+1) \end{bmatrix}, \quad E_{n+1/2} = \begin{bmatrix} \hat{\mathbf{T}}(n+1, n) & . \\ \hat{\mathbf{R}}(n+1, n) & . \end{bmatrix},$$
$$D_{n+1/2} = \begin{bmatrix} I & \mathbf{R}_{n+1/2} \\ . & \mathbf{T}_{n+1/2} \end{bmatrix} \tag{4.4}$$

into $2m \times 2m$ matrices. The circumflex accents are used to imply modification by multiple reflection of unimbedded cell matrices. The six $2m \times 2m$ matrices given in the decomposition (4.4), with a suitable reinterpretation of the symbols used, appear in the work of van de Hulst (1963), p. 61. In the next stage of decomposition we find that

$$\mathbf{R}(1, n+1) = \begin{bmatrix} . & R(1, n)\hat{T}(n, n+1) \\ . & R(1, n+1) \end{bmatrix}, \quad \hat{\mathbf{T}}(n, n+1) = \begin{bmatrix} . & I \\ . & \hat{T}(n, n+1) \end{bmatrix}, \tag{4.5}$$

$$\mathbf{R}_{n+1/2} = \begin{bmatrix} . & R(1, n)T_{n+1/2} \\ . & R_{n+1/2} \end{bmatrix}, \quad \hat{\mathbf{T}}_{n+1/2} = \begin{bmatrix} I & . \\ . & T_{n+1/2} \end{bmatrix}, \tag{4.6}$$

$$\mathbf{R}(n+1, n) = \begin{bmatrix} . & . \\ . & \hat{R}(n+1, n) \end{bmatrix}, \quad \hat{\mathbf{T}}(n+1, n) = \begin{bmatrix} . & T_{n+1/2'} \\ . & \hat{T}(n+1, n) \end{bmatrix}. \tag{4.7}$$

As a result of this decomposition, certain equations are found to be redundant. If we write

$$V_{n+1/2} = \begin{bmatrix} \mathbf{V}_{n+1/2^+} \\ \mathbf{V}_{n+1/2^-} \end{bmatrix}, \quad \mathbf{V}_{n+1/2^+} = \begin{bmatrix} v_{n+1/2^+} \\ V_{n+1/2^+} \end{bmatrix}, \quad \mathbf{V}_{n+1/2^-} = \begin{bmatrix} . \\ V_{n+1/2^-} \end{bmatrix} \tag{4.8}$$

(using the fact that $v_{n+1/2^-}$ is always zero), we find that the actual computation can be written as follows. With the initial conditions $R(1, 1) = 0$ and $V_{1/2^+} = u_1^+$ we form successively

$$\begin{aligned} T_{n+1/2} &= [I - R(n+1, n)R(1, n)]^{-1}, \\ R_{n+1/2} &= T(n+1, n)R(1, n)T_{n+1/2}, \\ R(1, n+1) &= R(n, n+1) + R_{n+1/2}T(n, n+1), \\ \hat{T}(n, n+1) &= T_{n+1/2}T(n, n+1), \end{aligned} \tag{4.9}$$

and

$$\begin{aligned} T_{n+1/2'} &= [I - R(1, n)R(n+1, n)]^{-1}, \\ \hat{T}(n+1, n) &= T(n+1, n)T_{n+1/2'}, \\ \hat{R}(n+1, n) &= R(n+1, n)T_{n+1/2'}, \end{aligned}$$

with

$$\begin{aligned} V_{n+1/2^+} &= \hat{T}(n+1, n)V_{n-1/2^+} + [\Sigma_{n+1/2^+} + R_{n+1/2}\Sigma_{n+1/2^-}], \\ V_{n+1/2^-} &= \hat{R}(n+1, n)V_{n-1/2^+} + T_{n+1/2}\Sigma_{n+1/2^-}, \end{aligned} \tag{4.10}$$

for $n = 1, 2, \ldots, N$, successively. Then we form

$$\begin{aligned} u_{n+1^+} &= R(1, n+1)u_{n+1^-} + V_{n+1/2^+}, \\ u_{n^-} &= \hat{T}(n, n+1)u_{n+1^-} + V_{n+1/2^-}, \end{aligned} \tag{4.11}$$

for $n = N, N-1, \ldots, 1$, starting with the given value of u_{N+1^-}. These equations

show up the physical meaning of the $m \times m$ matrices. The notation has been chosen so that T denotes transmission, and R reflection operators: for example $T(n+1, n)$ is the transmission of the isolated layer for radiation in the positive direction incident on the face n. The corresponding transmission operator $\hat{T}(n+1, n)$ contains a factor $T_{n+1/2}'$ which, if expanded in a series,

$$T_{n+1/2}' = I + R(1, n)R(n+1, n) + R(1, n)R(n+1, n)R(1, n)R(n+1, n) + \ldots,$$

can be seen to take account of multiple diffuse reflections of positively directed radiation incident on face n between the layer $(n+\frac{1}{2})$ and the composite layer between faces 1 and n. We can construct equivalent interpretations for other operators.

We have omitted certain equations from the decomposition, namely those for $v_{n+1/2}{}^{+}$ and $u_n{}^{+}$. These are

$$v_{n+1/2}{}^{+} = T_{n+1/2}'V_{n-1/2}{}^{+} + R(1, n)T_{n+1/2}\Sigma_{n+1/2}{}^{-},$$

(and we remark that

$$V_{n+1/2}{}^{+} = T(n+1, n)v_{n+1/2}{}^{+} + \Sigma_{n+1/2}{}^{+})$$

and

$$u_n{}^{+} = R(1, n)\hat{T}(n, n+1)u_{n+1}{}^{-} + v_{n+1/2}{}^{+}.$$

The last equation can be shown to be equivalent to the first of equations (4.11).

To complete our description of the method of solution, we give a brief indication of what happens as we let the cell thickness tend to zero. In the limit (4.9) gives

$$\frac{dR(\tau)}{d\tau} = \Gamma^{+-}(\tau) - R(\tau)\Gamma^{--}(\tau) - \Gamma^{++}(\tau)R(\tau) + R(\tau)\Gamma^{-+}(\tau)R(\tau). \tag{4.12}$$

The first of equations (4.10) gives

$$\frac{dV^{+}(\tau)}{d\tau} = [R(\tau)\Gamma^{-+}(\tau) - \Gamma^{++}(\tau)]V^{+}(\tau) + S^{+}(\tau) + R(\tau)S^{-}(\tau). \tag{4.13}$$

The last of equations (4.11) gives

$$-\frac{du^{-}(\tau)}{d\tau} = [\Gamma^{-+}(\tau)R(\tau) - \Gamma^{--}(\tau)]u^{-}(\tau) + S^{-}(\tau) + \Gamma^{-+}(\tau)V^{+}(\tau) \tag{4.14}$$

and the second gives

$$u^{+}(\tau) = R(\tau)u^{-}(\tau) + V^{+}(\tau). \tag{4.15}$$

In these equations, which were first derived by other arguments by Rybicki & Usher (1966), we have

$$\Gamma^{+-}(\tau) = \tfrac{1}{2}\omega(\tau)M^{-1}p^{+-}(\tau)c, \quad \Gamma^{++}(\tau) = M^{-1}[I - \tfrac{1}{2}\omega(\tau)p^{++}(\tau)c], \tag{4.16}$$

with similar definitions for $\Gamma^{-+}(\tau)$ and $\Gamma^{--}(\tau)$. Also

$$S^{+}(\tau) = S^{-}(\tau) = M^{-1}[1 - \omega(\tau)]B(\tau). \tag{4.17}$$

The remaining equations give essentially nothing new.

5. *Numerical example.* The explicit solution of the last section has been programmed in FORTRAN and used to solve a variety of simple problems to test the capabilities of the method. For many problems one only wishes to know, say, the mean intensity or net flux distributions and in such case a low order of angular resolution is permissible, $m = 2$ or 3, say. If, however, one is interested in the

angular distributions themselves, a larger value of m is needed. In the problem we have used to illustrate the method, we have computed the intensity emerging from an isotropically scattering finite atmosphere, with constant albedo for single scattering. Solutions of this problem, in the form of the matrix

$$r = \tfrac{1}{2}R(\tau)c^{-1}, \tag{5.1}$$

where $R(\tau)$ is the matrix of equation (4.12), have been tabulated to six decimals by Bellman *et al.* (1963) for a set of Gaussian division points with $m = 7$ and various values of ω, for slabs of optical thickness up to 20. Essentially they integrated equation (4.12) using a fixed step Runge–Kutta procedure; they do not quote a step size, but taking account of exponential factors appearing in the solution suggests that they must have taken $\Delta\tau \ll \frac{1}{2}\mu_1$, where $\mu_1 \approx 0{\cdot}025$ is the smallest cosine occurring for $m = 7$. We have found this to be a necessary restriction when using the same method of solving equation (4.12) ourselves.

We can calculate the solutions required in two ways. Either we can use equation (4.9) as it stands, or else we can solve a sequence of problems with u_1^+ having a single non-zero element in, say, the m_0th position and with $u_{N+1}^- = 0$. This gives us a single column of the matrix for each choice of m_0 and fixed optical thickness. We used steps of 0·05, and with the ' diamond ' choice of weights in equation (2.18), we found that the two procedures agreed to the number of figures printed out by the computer. Our results agree closely with the tables given by Bellman *et al.*, as the selected results printed in Table I will confirm. The agreement is worst for small optical thicknesses, about 1 part in 10^4 in the case $\omega = 0{\cdot}5$, $\tau = 0{\cdot}2$. In the case of $\omega = 1$, $\tau = 5$, the solutions agree to six digits.

We shall report other calculations that we have made in due course.

6. *Discussion.* We have described the invariant S_n equations and shown how they may be used to solve quite general plane-parallel problems. However, we need more information about the numerical analysis of the method, and about its practical convenience as a tool for astrophysicists. We need far more space for these matters than is available here and we shall therefore give only the briefest outline of what is known.

To begin with, we have indicated that the method of solution embodied in equations (4.9)–(4.11) converges to the Rybicki–Usher equations (4.12)–(4.15). These are equivalent to the original system (2.1), and it is also possible to confirm that the difference equations (2.10) are consistent with equation (2.1). Next, it can be shown that the solution of the system (4.9)–(4.11) exists under quite general assumptions. It is in fact sufficient that

$$\|R(n, n+1) + T(n, n+1)\|_F \leqslant 1$$

$$\|R(n+1, n) + T(n+1, n)\|_F \leqslant 1,$$

where the modified norm, $\|A\|_F = \|(Mc)A(Mc)^{-1}\|$, in the sense of equation (2.17), and we have found these conditions to be satisfied in all the cases we have examined so far, whatever the step size, for $\omega \leqslant 1$. The reflection operators defined in these equations are always represented by non-negative matrices and so are the transmission operators, provided the cell thickness $\Delta\tau$ is restricted; it is sufficient that

$$\Delta\tau < \min_i \{\mu_i/[(1-X)(1-\tfrac{1}{2}\omega p_{ii}^{++}c_i)]\} = \tau_b.$$

TABLE I

Results of invariant S_n calculation of the matrix r of equation (5.1)

The matrix elements $r_{ij} \equiv r(\mu_i, \mu_j)$ are tabulated for values of μ which are given below to five decimal places:

$i =$	1	2	3	4	5	6	7
$\mu_i =$	0·02545	0·12923	0·29708	0·50000	0·70292	0·87077	0·97455
$\cos^{-1}\mu_i \approx$	88·5°	82·6°	72·7°	60·0°	45·3°	29·5°	13·0°

Asterisked elements are those showing the largest deviation from the results of Bellman *et al.* (1963). The magnitude of this deviation is printed below each matrix.

Case (a) $\omega = 0{\cdot}5$, $\tau = 0{\cdot}2$, $\Delta\tau = 0{\cdot}05$

j/i	1	2	3	4	5	6	7
1	0·06570	0·02255	0·01101	0·00681	0·00493	0·00401	0·00360
2	0·11454	0·06755	0·03860	0·02524	0·01873	0·01543	0·01392
3	0·12858	0·08872	0·05299	0·03518	0·02628	0·02172	0·01961
4	0·13381	0·09766	0·05921	0·03951	0·02957	0·02447	0·02210
5	0·13617	0·10187	0·06217	0·04157	0·03115	0·02578	0·02330
6	0·13732	0·10398	0·06366	0·04261	0·03194	0·02644	0·02389
7	0·13784*	0·10494	0·06433	0·04308	0·03230	0·02674	0·02417

Maximum deviation 7×10^{-5}.

Case (b) $\omega = 1{\cdot}0$, $\tau = 0{\cdot}5$, $\Delta\tau = 0{\cdot}05$

j/i	1	2	3	4	5	6	7
1	0·14060	0·05279	0·02796	0·01809	0·01341	0·01105	0·00997
2	0·26809	0·18160	0·11922	0·08372	0·06438	0·05402	0·04913
3	0·32640	0·27406	0·20244	0·14933	0·11746	0·09966	0·09108
4	0·35546	0·32392	0·25133	0·18918	0·15017	0·12799	0·11721
5	0·37046	0·35018	0·27792	0·21112	0·16829	0·14371	0·13173
6	0·37830	0·36400	0·29210	0·22290	0·17803	0·15218	0·13956
7	0·38196	0·37048	0·29879	0·22846	0·18264	0·15619	0·14326*

Maximum deviation 5×10^{-5}.

Case (c) $\omega = 1{\cdot}0$, $\tau = 5{\cdot}0$, $\Delta\tau = 0{\cdot}05$

j/i	1	2	3	4	5	6	7
1	0·14356	0·05651	0·03300	0·02407	0·01982	0·01760	0·01654
2	0·28698	0·20539	0·15155	0·12197	0·10520	0·09560	0·09080
3	0·38522	0·34838	0·30397	0·26889	0·24420	0·22814	0·21952
4	0·47303	0·47191	0·45257	0·42753	0·40437	0·38668	0·37633
5	0·54754	0·57219	0·57781	0·56848	0·55259	0·53721	0·52717
6	0·60235	0·64416	0·66870	0·67342	0·66549	0·65364	0·64478
7	0·63364	0·68475	0·72014	0·73352	0·73089	0·72164	0·71378

Maximum deviation $< 10^{-6}$.

The bound τ_b is infinite if $X = 1$ ('step' weighting), it can also be large if the scattering phase function is strongly peaked in the forward direction. The truncation error is reduced by taking $X = \frac{1}{2}$ and, for this case, we have taken $\Delta\tau \lesssim 2\mu_1$ as our working restriction, although a larger cell thickness could be used without destroying the positivity of the transmission operator. The numerical work of the last section, which was done with $\Delta\tau \approx 2\mu_1$, shows that this cell size gives quite acceptable accuracy. This means that we could take $\Delta\tau \approx 0{\cdot}4$ in the case $m = 2$, say, provided this gave us sufficiently accurate results.

We have already mentioned that some of our matrix relations appear in treatments of radiative transfer employing invariance techniques. We have therefore

examined our difference equations for further evidence of invariance properties. It is not difficult to show that principles of invariance appear *as a consequence* of the matrix structure formulated in Section 3. This means that our difference equations are consistent in two senses: they converge to the original differential equations in the limit, and they satisfy invariance principles. This is a highly significant observation, for if our operators $R(n, n+1)$, $T(n, n+1)$, $R(n+1, n)$, $T(n+1, n)$ were exact and the source vectors Σ were exact, then we should get, with exact arithmetic, exact values of the solution vectors. However, the operators are only correct to first order in cell optical thickness and possess a truncation error. This gives rise to errors in the solution to which we must add arithmetical errors arising from matrix manipulation. We can reduce the resultant error in principle either by taking thinner cells, or by finding more accurate representations of the cell operators. In the former case we increase both the storage required and the time of execution. In the latter case, we may use imbedding methods to calculate the cell operators and source vectors for multilayered cells. This is relatively fast and economical on storage and should enable us to solve smaller problems with great accuracy or larger problems with economy of storage. We are currently endeavouring to assess the practical worth of this idea.

It is interesting to compare our method with the Riccati equation method of Rybicki & Usher (1966) to which it converges. In our method, apart from basic cell quantities, it is only necessary to store the vectors $V_{n+1/2}{}^{+}$, $V_{n+1/2}{}^{-}$ and matrices $R(1, n+1)$ and $\hat{T}(n, n+1)$ for $n = 1,2,\ldots, N$, requiring a total of $2m(m+1)N$ numbers. The solutions can be stored separately or allowed to overwrite the V's on the reverse sweep. It is possible to arrange the calculation so that a minimum of matrix multiplication is required. Taking the multiplication count as an estimator of the time used, we find that we need approximately $(9m^3+5m^2)N$ multiplications. For the Rybicki–Usher method we need only store $V^{+}(\tau)$ and $R(\tau)$ on the forward integration, a total of $m(m+1)N$ numbers. Basic cell quantities amount to the same as in our method. The work involved depends on the type of integration routine employed and the step size permitted within the limits set by the accuracy desired. For example, if a Kutta–Merson scheme is used, requiring five entries in the auxiliary routine per step, we find that $5(4m^3+7m^2)N$ multiplications are required. This is more than twice the number needed in our method for the same number of steps. As we have seen, we may be able to use a larger step size without sacrificing too much accuracy, since the Runge–Kutta step size is dictated by the most rapidly varying term in the solution.

It is only fair to the Rybicki–Usher method to remark that it can be made much faster in the special case of isotropic scattering, which is the case of all its applications so far. The right-hand side of the R-equation can be factorized, and all the remaining equations expressed in terms of a vector X, which alone need be stored. It then has a distinct advantage on storage over the invariant S_n scheme.

The reader will notice that the equation (3.6) is similar in structure to the equations solved by Feautrier (1964). This resemblance is superficial, in that no obvious physical meaning can be attached to Feautrier's matrices. Our method has much more in common with that of Rybicki & Usher, as we have just pointed out.

Finally, we remark that the Carlson techniques are not restricted to plane-parallel slabs. There seems no reason in principle why we should not apply a similar analysis to the transfer equation in other coordinate systems, although the equations will undoubtedly be much more complicated. We are currently working on this.

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APPENDIX

Cell operators. We begin with equations (3.5), which we may write in the form

$$\begin{bmatrix} G_{n+1/2}{}^{++} & -G_{n+1/2}{}^{+-} \\ -G_{n+1/2}{}^{-+} & G_{n+1/2}{}^{--} \end{bmatrix} U_{n+1/2} = \begin{bmatrix} Q & \cdot \\ \cdot & \cdot \end{bmatrix} U_{n-1/2} + \begin{bmatrix} \cdot & \cdot \\ \cdot & Q \end{bmatrix} U_{n+3/2} + \tau_{n+1/2}(1-\omega_{n+1/2}) S_{n+1/2}, \qquad \text{(A.1)}$$

where the vectors have dimension $6m$ and the submatrices dimension $3m$. The inverse of the matrix on the left will be denoted by H, and its component submatrices are

$$\begin{aligned} H^{++} &= (G^{++})^{-1}[I - P^{+-}P^{-+}]^{-1}, \\ H^{--} &= (G^{--})^{-1}[I - P^{-+}P^{+-}]^{-1}, \\ H^{+-} &= H^{++}P^{+-}, \\ H^{-+} &= H^{--}P^{-+}, \end{aligned} \qquad \text{(A.2)}$$

where

$$P^{+-} = G^{+-}(G^{--})^{-1}, \quad P^{-+} = G^{-+}(G^{++})^{-1}.$$

Thus comparing with equation (3.6), we see that

$$A_{n+1/2} = \begin{bmatrix} H_{n+1/2}{}^{++}Q & \cdot \\ H_{n+1/2}{}^{-+}Q & \cdot \end{bmatrix} \quad B_{n+1/2} = \begin{bmatrix} \cdot & H_{n+1/2}{}^{+-}Q \\ \cdot & H_{n+1/2}{}^{--}Q \end{bmatrix} \qquad \text{(A.3)}$$

and

$$\Sigma_{n+1/2} = \tau_{n+1/2}(1-\omega_{n+1/2}) \begin{bmatrix} (H_{n+1/2}{}^{++} + H_{n+1/2}{}^{+-})S_{n+1/2} \\ (H_{n+1/2}{}^{-+} + H_{n+1/2}{}^{--})S_{n+1/2} \end{bmatrix}, \qquad \text{(A.4)}$$

where

$$S_{n+1/2} = \begin{bmatrix} . \\ . \\ b_{n+1/2} \end{bmatrix}, \quad Q = \begin{bmatrix} . & I & . \\ . & . & . \\ . & . & . \end{bmatrix}.$$

Setting

$$G^{++} = \begin{bmatrix} I & . & . \\ I-X^+ & X^+ & -I \\ -M & M & \tau Z^+ \end{bmatrix},$$

$$G^{+-} = \begin{bmatrix} . & . & . \\ . & . & . \\ . & . & \tau Y^{+-} \end{bmatrix}, \tag{A.5}$$

where

$$Z^+ = [I-\tfrac{1}{2}\omega p^{++}c] = I-Y^{++},$$
$$Y^{+-} = \tfrac{1}{2}\omega p^{+-}c,$$

we find

$$(G^{++})^{-1} = \begin{bmatrix} I & . & . \\ I-\tau\Delta^+Z^+ & \tau\Delta^+Z^+ & \Delta^+ \\ I-\tau X^+\Delta^+Z^+ & -(I-\tau X^+\Delta^+Z^+) & X^+\Delta^+ \end{bmatrix}, \tag{A.6}$$

where $\Delta^+ = (M+\tau Z^+X^+)^{-1}$, and similarly for matrices with + and − superscripts interchanged. It is now straightforward to show that

$$\mathbf{T}(n+1, n) = H_{n+1/2}{}^{++}Q, \quad \mathbf{R}(n+1, n) = H_{n+1/2}{}^{-+}Q$$

have the form of equation (3.8) with

$$\begin{aligned} T_c(n+1, n) &= [I-r^{+-}r^{-+}]^{-1}t^+, \\ T(n+1, n) &= (X^+)^{-1}[T_c(n+1, n)-(I-X^+)], \\ R_c(n+1, n) &= r^{-+}T_c(n+1, n), \\ R(n+1, n) &= (X^-)^{-1}R_c(n+1, n), \end{aligned} \tag{A.7}$$

where

$$\begin{aligned} r^{+-} &= \tau X^+\Delta^+Y^{+-}, \\ t^+ &= I-\tau X^+\Delta^+Z^+. \end{aligned} \tag{A.8}$$

The expressions for $\mathbf{T}(n, n+1)$, $\mathbf{R}(n, n+1)$ follow by interchanging plus and minus superscripts. In the same way, we find that

$$\Sigma_{n+1/2} = \begin{bmatrix} \mathbf{\Sigma}_{n+1/2}{}^+ \\ \mathbf{\Sigma}_{n+1/2}{}^- \end{bmatrix}, \tag{A.9}$$

where

$$\mathbf{\Sigma}_{n+1/2}{}^+ = \begin{bmatrix} . \\ \Sigma_{n+1/2}{}^+ \\ \Sigma_{c,\,n+1/2}{}^+ \end{bmatrix}$$

and

$$\begin{aligned} \Sigma_{c,\,n+1/2}{}^+ &= \tau_{n+1/2}(1-\omega_{n+1/2})(I-r^{+-}r^{-+})^{-1}(S_{n+1/2}{}^+ + r^{+-}S_{n+1/2}{}^-), \\ \Sigma_{n+1/2}{}^+ &= (X^+)^{-1}\Sigma_{c,\,n+1/2}{}^+, \\ S_{n+1/2}{}^+ &= X^+\Delta^+b_{n+1/2}, \end{aligned}$$

with corresponding relations when plus and minus signs are interchanged.

These equations may be physically interpreted by noting that equation (A.8) defines first order approximations for diffuse reflection and transmission operators for a slab of thickness τX^+ (in the case when X^+ is a multiple of I). The inverse matrices such as $(I-r^{+-}r^{-+})^{-1}$ then account for the effect of multiple diffuse reflections across the whole cell.