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A Difference Scheme for Radiative Transfer[1]

BURTON WENDROFF

Department of Mathematics, University of Denver, Denver, Colorado 80210

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ABSTRACT

The numerical description of the state of matter which is in the presence of a radiation field, and which scatters, absorbs, and emits that radiation is far from straightforward. Three general methods have been applied to various problems: invariant imbedding, Monte Carlo, and direct discretization of the relevant integrodifferential equations. At the moment the last method seems to possess the greatest versatility and it also has had the most success. A special discrete, or finite difference method is discussed in this paper. We first present a set of requirements such as conservation and correct asymptotic behavior, which, although quite reasonable, cannot be satisfied by a finite difference method on a fixed word length machine. We then construct discrete equations which satisfy a set of relaxed requirements in an ideal situation, namely, without scattering and assuming local thermodynamic equilibrium. We also give some numerical results.

1. The special radiation transport problem we will consider concerns a material of unit density, at rest (all hydrodynamic effects ignored), which absorbs and emits but does not scatter radiation. The equation expressing conservation of photons is

$$\frac{1}{c}\frac{\partial I}{\partial t} + \boldsymbol{\omega} \cdot \nabla I = S - \sigma I \tag{1.1}$$

where $I = I(x, t, \boldsymbol{\omega}, \nu)$ is the specific photon intensity at space position $x = (x_1, x_2, x_3)$, time t, direction $\boldsymbol{\omega}$ and frequency ν. $\boldsymbol{\omega}$ is a unit vector or a point on the surface of the unit sphere, ∇ is the spatial gradient operator, $\sigma = \sigma(x, t, \nu)$ is the absorption coefficient. S is a source which we restrict to be σ times the Planck function

$$S = \sigma B(T, \nu) = \frac{2h\nu^3}{c^2}(e^{h\nu/kT} - 1)^{-1}\sigma$$

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Here, $T = T(x, t)$ is the temperature of the material. Note also that σ in general depends on T as well as explicitly on x and t.

An additional equation is needed to determine the temperature T. This equation expresses the conservation of total energy in the system. Putting

$$E_R = c^{-1} \iint I \mid d\omega \mid d\nu$$

$$\mathbf{F}_R = \iint I\omega \mid d\omega \mid d\nu$$

$$E_M = E_M(T) = \text{Material energy density}$$

we have

$$\frac{\partial E_M}{\partial t} = -\left(\frac{\partial E_R}{\partial t} + \operatorname{div} \mathbf{F}_R\right) \tag{1.2}$$

or equivalently

$$\frac{\partial Ew}{\partial t} = -\int_0^\infty \sigma \left[4\pi B(T, \nu) - \int I \mid d\omega \mid\right] d\nu \tag{1.3}$$

The equality of the right sides of the above can be seen by integrating (1.1).

A complete determination of I and T requires initial and boundary conditions. We assume that $I(x, 0, \omega, \nu)$ and $T(x, 0)$ are given initially and $I(x, t, \omega, \nu)$ is given at the boundaries for all incoming directions.

2. As we have seen in the previous section

$$\frac{\partial E_R}{\partial t} + \operatorname{div} \mathbf{F}_R = \iint (S - \sigma I) \mid d\omega \mid d\nu \tag{2.1}$$

This expresses the local conservation of radiant energy. The left side of (2.1) is the change in radiant energy in an infinitesimal space-time volume element, the right side is the change due to absorption and emission. Equations (1.2) and (1.3) say we have local thermodynamic equilibrium, that is, the change in radiant energy is exactly balanced by the change in material energy at each point. Theoretic, pragmatic, and aesthetic considerations lead us to require that in some sense both of the above conservation principles should have analogues in the finite difference scheme. This means that whatever discrete set-up is used for (1.1), summation over direction and frequency should produce an equation similiar in form to (2.1), that is, one expressing a local conservation of radiant energy; and the numerical value of either side of (2.1) should balance the numerical change in material energy density

by which the temperature is computed. Thus, conservation is one of the requirements imposed on the difference scheme.

The second requirement is not so evident but it is important. It concerns the behavior of the numerical solution for the limiting cases of very large or very small σ (compared to the dimensions of the system). In the former case the radiation diffusion approximation provides an accurate, efficient method of solution. We cannot expect our difference scheme to be as efficient, but we do have the right to ask it to be as accurate. This can only happen if our difference equations for large σ become essentially the same difference equations used in the diffusion approximation. A similar statement applies to the other limiting case.

The remaining requirements are positivity, accuracy, and stability. Since the intensity and temperature are positive in fact, it would be nice if the difference scheme could guarantee a positive solution. Accuracy refers to the truncation error of the scheme, which we would like to be of high order. Finally, since a stability condition is likely to involve the speed of light in an unpleasant way, we would prefer to have an unconditionally stable scheme.

No finite difference scheme on a machine with a finite word length can satisfy all the above conditions. First, the limiting behavior and conservation conditions are inconsistent. If we consider a thick (large σ) slab, the diffusion approximation says that

$$I = B - (\mu/\sigma)\frac{\partial B}{\partial x}$$

so that the right side of (2.1) is zero but the left is not. What actually happens in the computer is that because B is close to I, $\sigma(B - I)$ is all noise. In a thin slab I will be a constant depending on the direction plus a term of order σ. In this case the computation of $\operatorname{div}\mathbf{F}_R$ by differences will result in nothing but noise whereas the right side of (2.1) will be correct.

Second, we cannot have guaranteed positive intensities and also a high order of truncation error. Only a positive scheme, that is to say one in which new values are a positive linear combination of old values, is sure to have a positive solution given positive initial data. P. D. Lax [4] has shown that except in special not interesting cases positive schemes necessarily are the least accurate. We can, however, remove one glaring source of negative intensities, the term σI, in such a way as to maintain second order accuracy (corresponding to centered differences). In doing this the positivity of certain average intensities will be conserved. It is only when these averages are solved for the intensities at mesh points that anything can go negative. We call such a situation almost positive.

Our difference scheme will be locally and globally conservative, asymptotically correct if computed with infinitely many significant figures, almost positive, and

unconditionally stable. It is reasonably efficient as far as computer time is concerned, but it does require the preparation and storage of multi-dimensional tables.

3. The difference scheme is obtained by being careful about conservation in the left side of (1.1), and by being careful about asymptotic behavior in the right side, an idea first used by I. P. Grant [3].

Let

$$L = \frac{1}{c}\frac{\partial}{\partial t} + \boldsymbol{\omega} \cdot \nabla$$

Conservative difference approximations to the operator L have been obtained by Carlson and Lathrop [1] for arbitrary geometries. We will restrict our discussion to the slab, for which

$$L = \frac{1}{c}\frac{\partial}{\partial t} + \mu \frac{\partial}{\partial r}$$

and the sphere

$$L = \frac{1}{c}\frac{\partial}{\partial t} + \mu \frac{\partial}{\partial r} + \frac{1-\mu^2}{r}\frac{\partial}{\partial \mu}$$

The parameter μ varies from -1 to 1, and

$$\int I \mid d\boldsymbol{\omega} \mid = 2\pi \int_{-1}^{1} I \, d\mu$$

$$\int I\boldsymbol{\omega} \mid d\boldsymbol{\omega} \mid = 2\pi \int_{-1}^{1} I\mu \, d\mu$$

To obtain discrete operators $\bar{L}$ corresponding to the operators L, Carlson and Lathrop first introduce the following notation: for a given net of points (r_i, t_s, μ_m) and for any function $f(r_i, t_s, \mu_m)$ let

$$f_i = f(r_i, t_{s+1/2}, \mu_m)$$
$$f_s = f(r_{i+1/2}, t_s, \mu_m)$$
$$f_{m+1/2} = f(r_{i+1/2}, t_{s+1/2}, \mu_{m+1/2})$$

This avoids a proliferation of indices, but it does impose a burden on the reader. The Carlson and Lathrop difference operators are, for the slab,

$$\bar{L}I = \frac{I_{s+1} - I_s}{c\,\Delta t} + \mu_m \frac{I_{i+1} - I_i}{r_{i+1} - r_i} \tag{3.1}$$

and for the sphere,

$$\bar{L}I = \frac{I_{s+1} - I_s}{c\,\Delta t} + \mu_m \frac{A_{i+1}I_{i+1} - A_iI_i}{V_i} + \frac{\alpha_{m+1/2}I_{m+1/2} - \alpha_{m-1/2}I_{m-1/2}}{V_i w_m} \tag{3.2}$$

where

$$V_i = \frac{4\pi}{3}(r_{i+1}^3 - r_i)$$

$$A_i = 4\pi r_i^2$$

The μ_m are the direction cosines of the photon paths and are chosen symmetric about the origin. The weights w_m are taken to satisfy

$$\sum w_m = 2$$

$$\sum \mu_m w_m = 0 \tag{3.3}$$

$$\sum \mu_m^2 w_m = \tfrac{2}{3}$$

The $a_{m+1/2}$ are defined as follows

$$\alpha_{1/2} = \alpha_{M+1/2} = 0$$

$$\frac{\alpha_{m+1/2} - \alpha_{m-1/2}}{w_m} = -\mu_m(A_{i+1} - A_i) \tag{3.4}$$

Since $\mu_m < \mu_{m+1}$, and μ_1 is the most negative μ, the $a_{m+1/2}$ are all nonnegative.

In the next section we will introduce a suitable approximation for $S - \sigma I$, so that the difference equations become

$$\bar{L}I = S - \sigma I$$

We have more unknowns than equations, so additional conditions must be imposed. This can be done in two ways. The quantities I_i, I_s, $I_{m+1/2}$ represent average intensities on the faces $r = r_i$, $t = t_s$, $\mu = \mu_{m+1/2}$, respectively, of an elementary mesh cell. If we introduce the quantities

$$I(r_i, t_s, \mu_{m+1/2}) = I_{i,s,m+1/2}$$

and define

$$I_i = \tfrac{1}{4}[I_{i,s,m+1/2} + I_{i,s+1,m+1/2} + I_{i,s,m-1/2} + I_{i,s+1,m-1/2}] \tag{3.5}$$

and so on, then there are just enough equations to determine all the $I_{i,s+1,m+1/2}$,

given $I_{i,s,m+1/2}$ and the boundary conditions. If we adopt this procedure, it follows that

$$I_i + I_{i+1} = I_s + I_{s+1} = I_{m+1/2} + I_{m-1/2} \tag{3.6}$$

Alternatively, we may simply impose (3.6) as an extra set of conditions.

The operators $\bar{L}$ are conservative, for if we set

$$E_s(\nu) = \frac{2\pi}{c} \sum_m I_s w_m$$

$$F_i(\nu) = 2\pi \sum_m I_i \mu_m w_m$$

then for the sphere,

$$2\pi \sum_m \bar{L} I w_m = \frac{E_{s+1} - E_s}{\Delta t} + \frac{1}{V_i}(A_{i+1}F_{i+1} - A_i F_i)$$

Therefore,

$$2\pi \int_0^\infty \left(\sum_m \bar{L} I w_m \right) d\nu$$

is a conservative difference approximation for

$$\frac{\partial E_R}{\partial t} + \operatorname{div} \mathbf{F}_R$$

Conservation can be obtained in other ways, but this method has a property which is crucial for us. It follows from (3.4) that (for the sphere) if we set

$$\gamma = \frac{1}{c\,\Delta t} + \frac{\mu_m A_{i+1}}{V_i} + \frac{\alpha_{m+1/2}}{V_i w_m} \tag{3.7}$$

then

$$\gamma = \frac{1}{c\,\Delta t} + \frac{\mu_m A_i}{V_i} + \frac{\alpha_{m-1/2}}{V_i w_m} \tag{3.8}$$

As a result of this we have

$$\bar{L} I = \gamma (I_P - I_Q) \tag{3.9}$$

where, I_P and I_Q are averages of the I's (linear combinations with non-negative coefficients adding to one). For example, if $\mu_m > 0$,

$$I_P = \gamma^{-1}\left[\frac{1}{c\,\Delta t} I_{s+1} + \frac{\mu_m A_{i+1}}{V_i} I_{i+1} + \frac{\alpha_{m+1/2}}{V_i w_m} I_{m+1/2}\right] \tag{3.10}$$

$$I_Q = \gamma^{-1}\left[\frac{1}{c\,\Delta t} I_s + \frac{\mu_m A_i}{V_i} I_i + \frac{\alpha_{m-1/2}}{V_i w_m} I_{m-1/2}\right] \tag{3.11}$$

A similar statement holds, trivially, for the slab. We will exploit (3.9) in the following section.

4. In the absence of scattering equation (1.1) can be integrated by introducing the characteristic parameter s, where $d/ds = (1/c)(\partial/\partial t) + \omega \cdot \nabla$, so that

$$I(s) = I(0) \exp\left[-\int_0^s \sigma\, ds'\right] + \int_0^s \sigma B \exp\left[-\int_{s'}^s \sigma\, ds''\right] ds'$$

Let Q be some point in (r, μ, t) space. Put $s(Q) = 0$ and measure off along the characteristic through Q a positive length Δs. Then

$$\int_0^{\Delta s} \sigma(B - I)\, ds = I(0)\left\{\exp\left[-\int_0^{\Delta s} \sigma\, ds\right] - 1\right\} + \int_0^{\Delta s} \sigma B \exp\left[-\int_s^{\Delta s} \sigma\, ds'\right] ds \tag{4.1}$$

We now replace

$$S - \sigma I = \sigma(B - I)$$

by

$$\frac{1}{\Delta s}\int_0^{\Delta s} \sigma(B - I)\, ds$$

and in addition we put

$$\begin{aligned} \Delta s &= \gamma^{-1} \\ I(0) &= I_Q \end{aligned} \tag{4.2}$$

so that from

$$\bar{L}I = \frac{1}{\Delta s}\int_0^{\Delta s} \sigma(B - I)\, ds$$

we get

$$I_P = I_Q \exp\left[-\int_0^{\Delta s} \sigma\, ds\right] + \int_0^{\Delta s} \sigma B \exp\left[-\int_s^{\Delta s} \sigma\, ds'\right] ds \tag{4.3}$$

Equation (4.3) together with either (3.5) or (3.6) constitutes the basic difference scheme. The related problems of frequency discretization and the approximation of the integrals which appear in (4.3) are discussed in the next section.

The equations (4.2) are what enabled us to tie together the approximations of the left and right sides of (1.1). The motivation for them is given in Figure 4.1. The line C is the characteristic corresponding to $\mu = \mu_m > 0$ which passes through the center of the mesh cell, for slab geometry. In this case the length of the segment PQ is γ^{-1}.

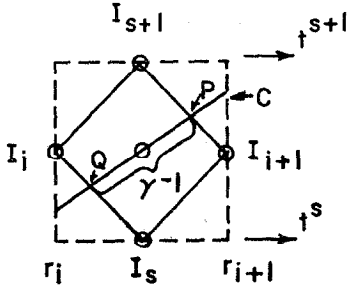

FIG. 4.1

If in addition we define $I(P)$ by linear interpolation on I_{s+1}, I_{i+1}, and if we define $I(Q)$ correspondingly, then it turns out that

$$I(P) = I_P$$
$$I(Q) = I_Q$$

Thus, for the slab the equations (4.2) are exact for a suitable choice of Q. In the sphere these relations are only approximately satisfied, but with a degree of accuracy consistent with the overall accuracy of the scheme.

5. The integrals in the difference scheme are evaluated by assuming the following approximate form σ and B:

$$\sigma(s) = \begin{cases} \sigma_L, & 0 \leqslant s \leqslant \Delta s/2 \\ \sigma_R, & \Delta s/2 \leqslant s \leqslant \Delta s \end{cases}$$

$$B(s) = \begin{cases} B_L + D_L s, & 0 \leqslant s \leqslant \Delta s/2 \\ B_R + D_R(s - \Delta s), & \Delta s/2 \leqslant s \leqslant \Delta s \end{cases}$$

We then write

$$\int_0^{\Delta s} \sigma B \exp\left[-\int_s^{\Delta s} \sigma\, ds'\right] ds = \int_0^{\Delta s/2} \sigma_L B(s) \exp[-\sigma_L(\Delta s - s)]\, ds + \int_{\Delta s/2}^{\Delta s} \sigma_R B(s) \exp[-\sigma_R(\Delta s - s)]\, ds$$

The first term above is not correct, but the correct expression would cause the functions q_i defined later in this section to depend on two values of T instead of just one. That complication would make this method impractical. We now have

$$\int_0^{\Delta s} \sigma B \exp\left[-\int_0^{\Delta s} \sigma\, ds'\right] ds$$

$$= B_R\left[1 - \exp\left(-\sigma_R \frac{\Delta s}{2}\right)\right]$$

$$+ D_R\left[\frac{\Delta s}{2}\exp\left(-\sigma_R \frac{\Delta s}{2}\right) - \frac{1}{\sigma_R}\left(1 - \exp\left(-\sigma_R \frac{\Delta s}{2}\right)\right)\right]$$

$$+ B_L\left[\exp\left(-\sigma_L \frac{\Delta s}{2}\right) - \exp(-\sigma_L\, \Delta s)\right]$$

$$+ D_L\left[\frac{\Delta s}{2}\exp\left(-\sigma_L \frac{\Delta s}{2}\right) - \frac{1}{\sigma_L}\left(\exp\left(-\sigma_L \frac{\Delta s}{2}\right) - \exp(-\sigma_L\, \Delta s)\right)\right] \quad (5.1)$$

At this point we discretize the continuous frequency parameter ν. One way of doing this is to introduce discrete values ν_g,

$$0 = \nu_0 < \nu_1 < \cdots < \nu_G$$

and to define

$$I^g = \int_{\nu_g}^{\nu_{g+1}} I\, d\nu$$

From (4.3) we obtain

$$I_P{}^g = \int_{\nu_g}^{\nu_{g+1}} I_Q \exp\left[-\int_0^{\Delta s} \sigma\, ds\right] d\nu + \int_{\nu_g}^{\nu_{g+1}} \int_0^{\Delta s} \sigma B \exp\left[-\int_s^{\Delta s} \sigma\, ds'\right] ds\, d\nu$$

The easiest thing to assume here is that $I(\nu)$ is constant in the interval $[\nu_g, \nu_{g+1}]$, and $I(\nu) = 0$, $\nu > \nu_G$. Then

$$I_P{}^g = I_Q{}^g(\nu_{g+1} - \nu_g)^{-1} \int_{\nu_g}^{\nu_{g+1}} \exp\left[-\int_0^{\Delta s} \sigma\, ds\right] d\nu + \int_{\nu_g}^{\nu_{g+1}} \int_0^{\Delta s} \sigma B \exp\left[-\int_s^{\Delta s} \sigma\, ds'\right] ds\, d\nu \quad (5.2)$$

No further approximations with respect to frequency need be made since all integrations in (5.1) can be performed using (5.2) once the arguments T and Δs are specified. We first note that D (meaning D_L or D_R) represents dB/ds. Then

$$D = \frac{dB}{ds} = \frac{dT}{ds}\frac{\partial B}{\partial T}$$

In order to have the equations be correct in the thick limit we replace dT/ds by

$$\bar{D} = \frac{1}{4T^3}\frac{dT^4}{ds}$$

Now, let

$$q_0 = \int B(T)\left[1 - \exp\left(-\sigma(T)\frac{\Delta s}{2}\right)\right] d\nu$$

$$q_1 = \int \frac{\partial B}{\partial T}\left[\frac{\Delta s}{2}\exp\left(-\sigma\frac{\Delta s}{2}\right) - \sigma^{-1}\left(1 - \exp\left(-\sigma\frac{\Delta s}{2}\right)\right)\right] d\nu$$

$$q_2 = \int B\left[\exp\left(-\sigma\frac{\Delta s}{2}\right) - \exp(-\sigma\,\Delta s)\right] d\nu$$

$$q_3 = \int \frac{\partial B}{\partial T}\left[\frac{\Delta s}{2}\exp\left(-\sigma\frac{\Delta s}{2}\right) - \sigma^{-1}\left[\exp\left(-\sigma\frac{\Delta s}{2}\right) - \exp(-\sigma\,\Delta s)\right]\right] d\nu$$

$$q_4 = \frac{1}{\Delta\nu}\int e^{-\sigma\Delta s}\, d\nu$$

We now make the correspondence

$$P \leftrightarrow R$$
$$Q \leftrightarrow L$$

in (5.1). Let $q_k(P)$, $k = 0, 1, 2, 3$ be the functions q_k "evaluated" at P, and let $q_4(P, Q)$ be q_4 "evaluated" at the cell center. These quantities are not well defined at this time, since we do not know how to associate a temperature T with P. Just how these evaluations are to be made will be specified in the next section. The difference equations become

$$\begin{aligned} I_P{}^g &= q_4(P, Q)\, I_Q{}^g + q_0(P) + \bar{D}_P q_1(P) + q_2(Q) + \bar{D}_Q q_3(Q) \\ &\equiv \alpha I_Q{}^g + \beta_1(P) + \beta_2(Q) \end{aligned} \tag{5.3}$$

together with (3.5) or (3.6). The energy balance equation becomes

$$2\pi\, V\Delta t \sum_m \sum_g (\bar{L}I^g)\, w_m = -\int_{\text{space-time cell}} \frac{\partial E_M}{\partial t}\, dV\, dt \tag{5.4}$$

If we subtract $I_Q{}^g$ from both sides of (5.3) we see that, modulo the various approximating assumptions that have been made,

$$2\pi \sum_g \sum_m (\bar{L}I^g)\, w_m = 2\pi \int_0^\infty d\nu \sum_m \frac{w_m}{\Delta s}\int_0^{\Delta s} \sigma(B - I)\, ds \tag{5.5}$$

We have already seen that the left side of (5.5) well represents the left side of (2.1). It is clear that the right side of (5.5) also represents the right side of (2.1). Thus, our scheme satisfies the first conservation principle. By (5.4) it also satisfies the second.

The difference scheme is almost positive in the sense that if I_Q^g is positive, then so will be I_P^g. The quantities I_i^g, I_s^g, $I_{m+1/2}^g$ obtained from (3.10) and (3.6) could be negative if there is too much variation in I^g from one mesh point to the next, that is if the mesh is too coarse.

The accuracy and stability are difficult to assess rigorously because of the complexity and nonlinearity of the equations. The lower order terms in (1.1) and the frequency dependence of I have been treated rather crudely. However, the derivatives appearing in (1.1) have been replaced by centered differences in an unconditionally stable way. This type of differencing has been discussed by the author in two previous publications, [5], and [6].

6. To determine the asymptotic behavior of the difference equations, consider first a thick sphere (or slab). We define this to mean that all terms involving

$$e^{-\sigma\Delta s}B,\ e^{-\sigma\Delta s}\frac{\partial B}{\partial T},\qquad \text{or}\qquad e^{-\sigma\Delta s}I^g$$

can be neglected. Then from (5.3),

$$I_P^g = q_0(P) + \bar{D}_P q_1(P)$$

where now

$$q_0 = \int B(T)\,d\nu$$

$$q_1 = -\int \frac{1}{\sigma(T)}\frac{\partial B}{\partial T}\,d\nu$$

Let f stand for any one of the functions β_1, β_2.

Let P_s, P_i, $P_{m+1/2}$ be the (r, t, μ) points corresponding to I_s, I_i, $I_{m+1/2}$, and let $P^s_{i,m+1/2} = (r_i, t_s, \mu_{m+1/2})$.

Now I_P^g is defined as a linear combination of the I^g at certain mesh points, for example,

$$I_P^g = aI_{s+1}^g + bI_{i+1}^g + cI_{m+1/2}^g$$

We define $f(P)$ in (5.3) as the same linear combination.

$$f(P) = af(P_{s+1}) + bf(P_{i+1}) + cf(P_{m+1/2}) \tag{6.1}$$

We impose the auxiliary conditions (3.6) on $f(P_s)$, etc., by introducing quantities $f(P^s_{i,m+1/2})$ in such a way that

$$\begin{aligned} f(P_{s+1}) &\equiv \tfrac{1}{4}[f(P^{s+1}_{i+1,m+1/2}) + f(P^{s+1}_{i,m+1/2}) + f(P^{s+1}_{i,m-1/2}) + f(P^{s+1}_{i+1,m-1/2})] \\ f(P_{i+1}) &\equiv \tfrac{1}{4}[f(P^{s+1}_{i+1,m+1/2}) + f(P^{s}_{i+1,m+1/2}) + f(P^{s+1}_{i+1,m-1/2}) + f(P^{s}_{i+1,m-1/2})] \quad (6.2) \\ f(P_{m+1/2}) &\equiv \tfrac{1}{4}[f(P^{s+1}_{i+1,m+1/2}) + f(P^{s}_{i+1,m+1/2}) + f(P^{s+1}_{m,i+1/2}) + f(P^{s}_{i,m+1/2})] \end{aligned}$$

We now define the functions $f(P^s_{i,m+1/2})$. Note first that Δs is here a fixed function of (P, Q), that is, it is considered to be independent of (r, t, μ). The functions f still depend explicitly on (r, t, μ). For example, $\bar{D}$ depends on (r, t, μ). Now, we also fix those parameters which identify the matter in the cell (P, Q).

In defining the $f(P^s_{i,m+1/2})$ we assume that T is given at half-integer space points and integer times, $T = T^s_{i+1/2}$. We let

$$T_i{}^s = \tfrac{1}{2}(T^s_{i+1/2} + T^s_{i-1/2})$$

The definition of $f(P^s_{i,m+1/2})$ is as follows:

(a): Replace T by $T_i{}^s$ in $B(T)$, $\partial B/\partial T$, $\sigma(T)$

(b): Replace $\bar{D}$ by either

$$\frac{1}{4}(T_i{}^s)^{-3}\,\mu_{m+1/2}\,\frac{(T^s_{i+1/2})^4 - (T^s_{i-1/2})^4}{\Delta r} \tag{6.3}$$

or

$$\frac{1}{4}(T_i{}^s)^{-3}\left[\frac{(T_i{}^s)^4 - (T_i^{s-1})^4}{c\,\Delta t} + \mu_{m+1/2}\,\frac{(T^s_{i+1/2})^4 - (T^s_{i-1/2})^4}{\Delta r}\right] \tag{6.4}$$

In (6.4) we have used

$$\bar{D} = \frac{dT}{ds} = \frac{1}{4T^3}\frac{dT^4}{ds} = \frac{1}{4T^3}\left[\frac{1}{c}\frac{\partial T^4}{\partial t} + \mu\frac{\partial T^4}{\partial r}\right]$$

In (6.3) we have dropped $(1/c)(\partial T^4/\partial t)$, which will lead to the usual diffusion approximation.

Although it doesn't appear in the thick limit we must also define $q_4(P, Q)$. If we are integrating across the cell from r_i to r_{i+1}, t_s to t_{s+1}, then

$$q_4(P, Q) = q_4(\sigma_{i+1/2}(\tfrac{1}{2}T^{s+1}_{i+1/2} + \tfrac{1}{2}T^s_{i+1/2}))$$

It now follows by induction that

$$N^g_{s+1} = q_0(P_{s+1}) + \bar{D}_{P_{s+1}} q_2(P_{s+1})$$

and so on for

$$N^g_{i+1}\,,\ N^g_{m+1/2}\,.$$

There is no loss of generality in taking just one frequency interval. Suppressing g, and using (6.3) we have, with $a = 8\pi^5k^4/15c^3h^3$,

$$N_{s+1} = \frac{ac}{4\pi}\frac{1}{2}\left[(T^{s+1}_{i+1})^4 + (T^{s+1}_i)^4\right] - \frac{ac}{4\pi}\frac{1}{4}(\mu_{m+1/2} + \mu_{m-1/2})$$
$$\times\left[\frac{(T^{s+1}_{i+3/2})^4 - (T^{s+1}_{i+1/2})^4}{\bar\sigma_{i+1/2}(T^{s+1}_{i+1})\,\Delta r} + \frac{(T^{s+1}_{i+1/2})^4 - (T^{s+1}_{i-1/2})^4}{\bar\sigma_{i+1/2}(T^{s+1}_i)\,\Delta r}\right]$$

and

$$N_{i+1} = \frac{ac}{4\pi}\frac{1}{2}\left[(T^{s+1}_{i+1})^4 + (T^s_{i+1})^4\right] - \frac{ac}{4\pi}\frac{1}{4}(\mu_{m+1/2} + \mu_{m-1/2})$$
$$\times\left[\frac{(T^{s+1}_{i+3/2})^4 - (T^{s+1}_{i+1/2})^4}{\bar\sigma_{i+1\pm1/2}(T^{s+1}_{i+1})\,\Delta r} + \frac{(T^s_{i+3/2})^4 - (T^s_{i+1/2})^4}{\bar\sigma_{i+1\pm1/2}(T^s_{i+1})\,\Delta r}\right]$$
$$(\bar\sigma_{i+1/2} \quad \text{if} \quad \mu_m > 0, \qquad \bar\sigma_{i+3/2} \quad \text{if} \quad \mu_m < 0),$$

where $\bar\sigma$ is the Rosseland mean opacity

$$\bar\sigma_{i+1/2}(T) = \left[\int \frac{\partial B}{\partial T}(\sigma_{i+1/2}(T))^{-1}\,d\nu\right]^{-1}$$

There is no need to write $N_{m+1/2}$, for those terms cancel out of the energy balance equation. We thus have a discretization of the diffusion approximation,

$$N = \frac{ac}{4\pi}\left[T^4 - \frac{\mu}{\bar\sigma}\frac{\partial T^4}{\partial x}\right]$$

If we define

$$\mu_m = \tfrac{1}{2}(\mu_{m+1/2} + \mu_{m-1/2})$$

the reader can see that the energy balance equation becomes an implicit difference equation for the radiation diffusion equation.

The thin limit can be discussed in the case that I(incoming) $= 0$ at the boundaries. Then for small σ,

$$I_P{}^g = O(\sigma)$$

and therefore also $I_s{}^g$, $I_i{}^g$, and $I^g_{m+1/2}$ are $O(\sigma)$. Then

$$2\pi\,V\Delta t\sum_m\sum_g(\bar L I^g)\,w_m = 2\pi\,V\Delta t\sum_m\frac{w_m}{\Delta s}\int d\nu\int_0^{\Delta s}\sigma B\,ds + O(\sigma^2)$$

The first term on the left has the form $4\pi V \Delta t$ times an average σB, so the energy balance is

$$-\int_{\text{space–time cell}} \frac{\partial E_m}{\partial t}\, dt\, dV = 4\pi\, V\Delta t(\sigma B)_{\text{average}} + O(\sigma^2)$$

which is the correct form.

Note that both asymptotic limits will be correct only if exact arithmetic is used. In the thin limit the computation of $\bar{L}I^g = (\Delta_s)^{-1}(I_P{}^g - I_Q{}^g)$ will result in loss of significance due to cancellation of leading figures in the almost equal quantities $I_P{}^g$ and $I_Q{}^g$. In the thick limit we must compute $I_P{}^g = q_0(P) + \bar{D}_P q_1(P)$; since q_1 behaves like σ^{-1} it may be small compared to q_0 and so fixed word length addition could result in $I_P{}^g = q_0(P)$. This is completely wrong, for it is $\bar{D}_P q_1$ that enters into $\partial F/\partial r$ in the energy balance equation.

7. We turn now to some of the details of solving the difference equations. Suppose we are proceeding from time t_s to t_{s+1}. Then I_s, T^s are given.

(1) Guess a distribution T^{s+1}, say $T^{s+1} = T^s$, and compute all coefficients.

The transport difference equations are explicit in I when there is no scattering. Let the radii be

$$r_{i_0} < r_{i_0+1} \cdots < r_{i_1}$$

and let the angles be

$$-1 = \mu_{-M-1/2} < \mu_{-M+1/2} \cdots < \mu_{M+1/2}$$

(2) Solve the transport difference equations for $\mu = -1$. These are a special case of the equations already constructed, and are obtained from the equation

$$\frac{\partial I}{c\,\partial t} - \frac{\partial I}{\partial r} = \sigma(B - I)$$

using the mesh shown in Figure 7.1. Now, $I_{i+1}(i = i_1 - 1, m = -M)$ is given, so

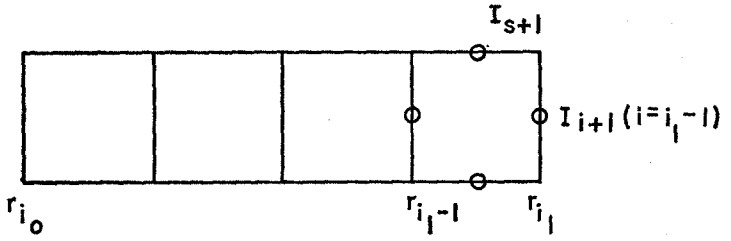

FIG. 7.1

there are two unknowns in that cell, I_{s+1} , I_i . These are determined from (4.3) and the equation

$$I_{s+1} + I_s = I_{i+1} + I_i$$

Then

$$2I_{m-1/2}(m = -M) \equiv I_{s+1} + I_s .$$

We then move in one cell and repeat the procedure.

(3) Compute I_{s+1} . *A* typical (r, t, μ) cell is shown in Figure 7.2. Start with $m = -M$, $i = i_1 - 1$. Then for the cell shown, I_s , I_{i+1} , $I_{m-1/2}$ are known. I_P will be a linear combination of I_{s+1} , I_i , $I_{m+1/2}$, so that (4.3) and the two auxiliary conditions determine I_{s+1} , I_i , and $I_{m+1/2}$. Repeat this for $i - 1$, $i - 2$,..., until $I_{i_0}(m = -M)$ has been found. Now advance m by one and repeat starting with $i = i_1 - 1$. When a positive μ is reached I_P will involve I_{s+1} , I_{i+1} , $I_{m+1/2}$. In that case I_{i_0} will be given, so start at the left end and sweep to the right.

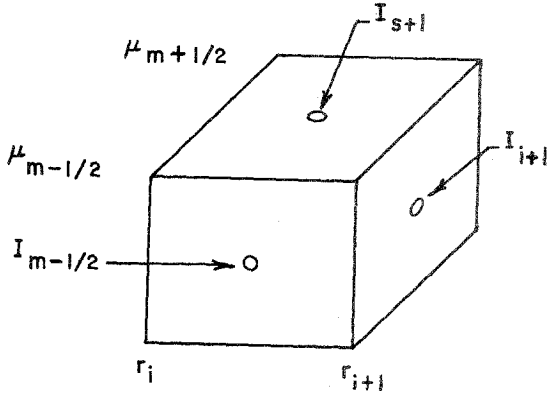

FIG. 7.2

(4) Correct T^{s+1}. The correction comes from the energy balance (5.4), which in difference form is

$$E_M(T^{s+1}_{i+1/2}) - E_M(T^s_{i+1/2}) + 2\pi\,\Delta t \sum_m \sum_g \bar{L} I^g w_m \equiv \mathscr{E}_{i+1/2} = 0$$

We consider three possible iterations.

Iteration A (Newton's Method). Choose a small number δ and define the matrix $\mathscr{E}'$ by

$$\mathscr{E}'_{ij} = \delta^{-1}[\mathscr{E}_{i+1/2}(T^{s+1}_{1/2},\ldots, T^{s+1}_{j+1/2} + \delta,\ldots) - \mathscr{E}_{i+1/2}(T^{s+1})]$$

then define $\hat{T}^{s+1}$ by

$$[\mathscr{E}'(\hat{T}^{s+1} - T^{s+1})]_{i+1/2} = -\mathscr{E}_{i+1/2}(T^{s+1})$$

and put $\hat{T}^{s+1} \to T^{s+1}$ and do (1), (2), (3).

This of course is a very time consuming iteration. Each column of $\mathscr{E}'$ requires a full solution of the transport difference equations. Some saving of time is possible since not all α's and β's need to be computed for each column. In the current model without scattering not all the intensities need to be computed either, but with scattering present this saving is not possible. It has also been suggested to us that modified Newton's Method might be effective, whetein $\mathscr{E}'$ is only re-computed intermittently.

Iteration B. This iteration takes advantage-of the explicit T dependence of the inhomogeneous terms in (5.3). Let

$$\beta(P, Q) = \beta_1(P) + \beta_2(Q)$$

Then

$$2\pi\, \Delta t \sum_m \sum_g (\bar{L} I^g)\, w_m = 2\pi\, \Delta t \sum_m \sum_g \left[\frac{\alpha - 1}{\Delta s} I_Q{}^g + \Delta s^{-1} \beta(P, Q)\right] w_m \tag{7.1}$$

Now, if we are in the cell $r_i < r < r_{i+1}$, then we can write

$$\beta(P, Q) = a^{g,m}_{i-1/2} T^{s+1}_{i-1/2} + b^{g,m}_{i+1/2} T^{s+1}_{i+1/2} + c^{g,m}_{i+3/2} T^{s+1}_{i+3/2} \tag{7.2}$$

as follows: in the functions q_k change variables from ν to $h\nu/kT$. This brings out a factor T^4 in q_0 and q_2, and a factor T^3 in q_1 and q_3, which cancels the T^{-3} in $\bar{D}$. Then write:

$$(T^{s+1}_{i+1/2})^4 = (T^{s+1}_{i+1/2})^3\, T^{s+1}_{i+1/2}$$

and put the cubic factor into $b^{g,m}_{i+1/2}$. Each $\bar{D}$ has a difference of fourth powers of T. Write these as a difference of T's times a cubic polynomial and put the cubics appropriately into $a^{g,m}_{i-1/2}$, etc. Let

$$a_{i-1/2} = 2\pi\, \Delta t \sum_m \sum_g (\Delta s)^{-1}\, a^{g,m}_{i-1/2} w_m \tag{7.3}$$

etc.

The iteration consists first of steps (1), (2), (3) with $\beta(P, Q)$ computed as written in (7.2). At the same time compute $a_{i-1/2}$, $b_{i+1/2}$, $c_{i+3/2}$. Now write the energy balance as

$$\begin{aligned} c_v(T^{s+1}_{i+1/2})\, \hat{T}^{s+1}_{i+1/2} + a_{i-1/2} \hat{T}^{s+1}_{i-1/2} + b_{i-1/2} \hat{T}^{s+1}_{i+1/2} \\ + c_{i+3/2} \hat{T}^{s+1}_{i+3/2} - E_m(T^s_{i+1/2}) + 2\pi\, \Delta t \sum_m \sum_g \frac{\alpha - 1}{\Delta s} I_Q{}^g w_m = 0 \end{aligned} \tag{7.4}$$

where

$$c_v = \frac{\partial E_m}{\partial T}$$

This system is easily solved by Gaussian elimination.

Iteration B has been observed to be convergent for both thick and thin problems, but it is most rapid for large σ. Presumably, an acceleration procedure could be used.

Iteration C (Simple Substitution). Here we simply put

$$\hat{T}^{s+1}_{i+1/2} = T^{s+1}_{i+1/2} - \frac{2\pi \Delta t}{c_v(T^{s+1})} \sum_m \sum_g \bar{L} I^g w_m$$

the radiation terms being computed from (1), (2), (3). Now put $\hat{T}^{s+1} \to T^{s+1}$ and repeat.

In a previous publication [7] we have shown how this iteration can easily fail.

As a final note in this section we should point out that the boundary cells require special treatment, since ΔT^4 is called for at cell boundaries. The easiest thing to do, although not physically satisfactory, is to simply extrapolate T^4.

8. We have attempted to test the frequency discretization used in our method on the following simple but nontrivial problem. A slab of finite thickness has radiation shining on it from one side. The absorption coefficient σ is a step function in frequency, with two steps. We wish to compare the steady-state temperature distribution computed with two frequency intervals and one interval.

The temperature T and frequency ν are replaced by dimensionless variables θ and u in such a way that the Planck function is now defined as

$$B(\theta, u) = \theta^4 u^3 (e^u - 1)^{-1}$$

The absorption has the following form

$$\sigma(u) = \begin{cases} 1, & 0 \leqslant u < 7.05/\theta \\ 100, & 7.05/\theta \leqslant u < \infty \end{cases}$$

The slab extends from $x = 0$ to $x = 8$. At $x = 0$ the incoming intensity is zero. The incoming intensity at $x = 8$ was obtained as follows. In [2], Carrier and Avrett compute the steady-state temperature distribution in a semi-infinite slab with the physical characteristics given above. Following a suggestion of *A.* Skumanich we assumed that θ^4 was linear from $x = 8$ to $x = \infty$ with slope and intercept read-off from the curve given in [2], namely

$$\theta(x = 8) = 3.28$$

$$\frac{d\theta^4}{dx}(x = 8) = 26$$

We then computed the incoming intensity at $x = 8$.

In Figure 8.1 we plot the results of Carrier and Avrett, a two frequency interval calculation and a one frequency interval calculation. In the latter case the cut-off frequency, ν_G was chosen so that

$$\frac{1}{\Delta\nu}\int e^{-\sigma\Delta s}\,d\nu \equiv \frac{1}{4}e^{-\Delta s} + \frac{3}{4}e^{-100\Delta s}$$

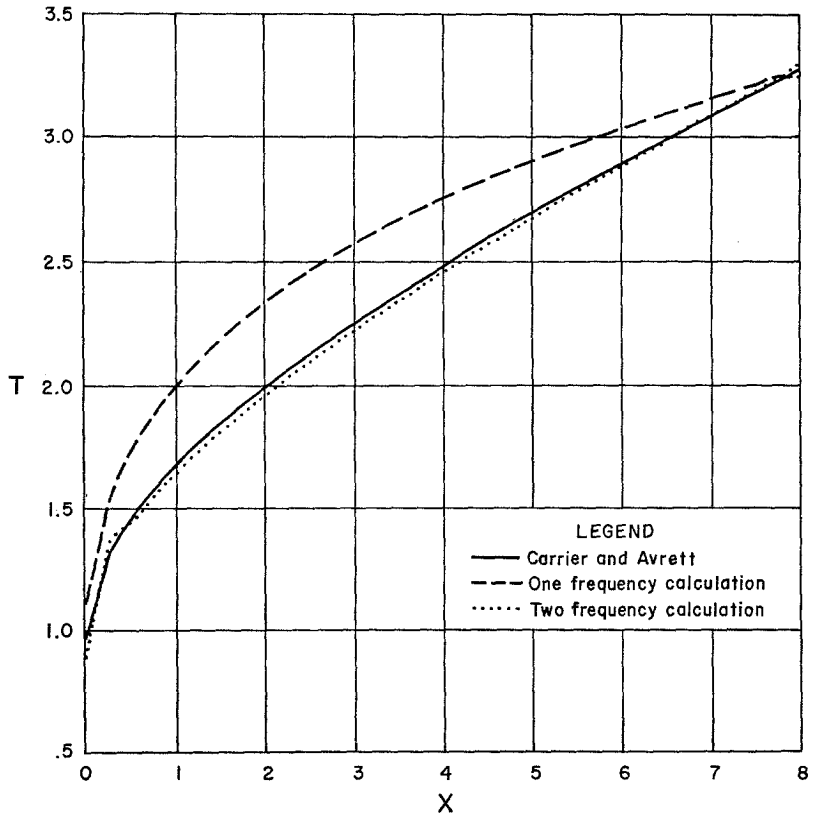

FIG. 8.1. This a relatively severe test because of the large jump in σ as a function of frequency, and one would not expect to obtain the complete temperature distribution very accurately using just one frequency interval.

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