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Analysis of a Monte Carlo Method for Nonlinear Radiative Transfer

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It has recently been proved that solutions of nonlinear radiative transfer problems satisfy a maximum principle (Andreev, Kozmanov, and Rachilov, *U.S.S.R. Comput. Math. Math. Phys.* **23**, 104 (1983); Mercier, *SIAM J. Math. Anal.*, in press). In this article it is shown that Monte Carlo solutions of such problems, obtained using the method of Fleck and Cummings (*J. Comput. Phys.* **8**, 313 (1971)), must satisfy this maximum principle for sufficiently small time-steps, but can violate it for sufficiently large time-steps. Analyses of the frequency-dependent and grey cases are given, and a numerical solution violating the maximum principle is discussed.

I. INTRODUCTION

A well-known method for obtaining Monte Carlo solutions of nonlinear radiative transfer problems is the algorithm proposed by Fleck and Cummings [3]. The basis of this method is conceptually straightforward: within each time-step, the nonlinear transport process is approximated by a linear one, which is solved by a standard linear transport Monte Carlo method. This algorithm contains implicit terms which lead to a "quasi-scattering" integral in the linearized transport process. However, because the algorithm is linear within each time-step, it cannot be fully implicit. In particular, opacities are evaluated at the old time-step, and the emission term is a product of quantities evaluated at the old and new time-steps. If the implicit terms are chosen judiciously, then one can conjecture that the algorithm is well behaved and stable for small time-steps, but since explicit terms are present, one should also conjecture that the solution might have unphysical behavior for

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sufficiently large time-steps. In this article we show that both these conjectures are true, and we describe the unphysical behavior in some detail.

Our primary analytical tool is a maximum principle which has recently been shown to hold for solutions of nonlinear radiative transfer problems [1, 2]. Specifically, we show that "ideal" solutions obtained by the Fleck–Cummings (FC) algorithm must satisfy this maximum principle for small time-steps, but may not satisfy it for large time-steps. By "ideal" solutions, we mean ones which are free of statistical Monte Carlo errors. Therefore, our analysis applies to the differential equations which the Monte Carlo method solves, but not to any specific Monte Carlo solution. However, in the "ideal" limit of an infinite number of particles and zero statistical error, our results do directly apply. The motivation for this article is that even though statistical fluctuations can cause any particular Monte Carlo solution to satisfy or violate the maximum principle, it is important to know whether or not the underlying equations have a solution which must satisfy this principle. In addition, these underlying equations have recently formed the basis of deterministic algorithms [4], and the analysis in this article can also be applied to this type of numerical methodology.

An outline of the remainder of this article follows. In Section 2 we introduce notation by describing the physical problem and stating the maximum principle for its solution. In Section 3 we describe the FC algorithm, and in Section 4 we state and prove its maximum principle. In Section 5 we discuss some variations of the FC algorithm, and in Section 6 we conclude with a brief discussion and a presentation of a numerical example which violates the maximum principle for large time-steps.

II. Statement of the Problem

In the absence of material motion, scattering, heat conduction, and internal sources, the equations of radiative transfer are [5]

$$\frac{1}{c}\frac{\partial I}{\partial t}+\mathbf{\Omega}\cdot\nabla I=\sigma(B-I), \tag{2.1}$$

$$\frac{\partial \mathscr{E}}{\partial t}=\iint \sigma(I-B)\,dv\,d\Omega, \tag{2.2}$$

with the initial conditions

$$I(\mathbf{x}, \mathbf{\Omega}, v, 0)=I_i(\mathbf{x}, \mathbf{\Omega}, v), \tag{2.3}$$

$$T(\mathbf{x}, 0)=T_i(\mathbf{x}), \tag{2.4}$$

and boundary condition

$$I(\mathbf{x}, \mathbf{\Omega}, v, t)=I_b(\mathbf{x}, \mathbf{\Omega}, v, t), \qquad \mathbf{x}\in\partial D, \mathbf{\Omega}\cdot\mathbf{n}<0. \tag{2.5}$$

In these equations, the unknowns are the specific intensity of radiation $I(\mathbf{x}, \mathbf{\Omega}, v, t)$ and the material temperature $T(\mathbf{x}, t)$. [Unless stated otherwise, $\mathbf{x}$ denotes position in the spatial domain $D \subset R^3$, $\mathbf{\Omega}$ is a unit vector in R^3 denoting direction, $v \in (0, \infty)$ denotes frequency, and $t > 0$ denotes time. Also, ∂D is the boundary of D, and $\mathbf{n}$ is the unit outer normal on ∂D.] The remaining known expressions, all positive, are c (the speed of light), $\sigma(v, T)$ (the opacity), $\mathscr{E}(T)$ (the material energy density), satisfying

$$\frac{\partial \mathscr{E}}{\partial T} = c_v > 0, \tag{2.6}$$

where $c_v(T)$ is the material heat capacity, and the Planck function

$$B(v, T) = \frac{2hv^3}{c^2} (e^{hv/kT} - 1)^{-1}, \tag{2.7}$$

where h is Planck's constant and k is Boltzmann's constant. B can easily be shown to satisfy, for all $v > 0$ and $T > 0$,

$$\frac{\partial^n B}{\partial T^n} > 0, \qquad n = 1, 2. \tag{2.8}$$

Finally, we define the equilibrium energy density $\phi(\mathbf{x}, t)$ and the radiation constant a by

$$\phi = \iint B \, dv \, d\Omega = acT^4, \tag{2.9}$$

$$a = \frac{8\pi^5 k^4}{15h^3 c^3}. \tag{2.10}$$

The problem posed by (2.1)–(2.5) is linear in I, but in general, highly nonlinear in T. Under constraints on σ and $\mathscr{E}$, it is known [1, 2] that this problem has a solution which satisfies the following:

MAXIMUM PRINCIPLE. *Let $0 \leqslant T_L < T_U$ be fixed constants, and let I_i, T_i, and I_b satisfy*

$$B(v, T_L) \leqslant I_i(\mathbf{x}, \mathbf{\Omega}, v) \leqslant B(v, T_U), \tag{2.11}$$

$$T_L \leqslant T_i(\mathbf{x}) \leqslant T_U, \tag{2.12}$$

and

$$B(v, T_L) \leqslant I_b(\mathbf{x}, \mathbf{\Omega}, v, t) \leqslant B(v, T_U), \qquad \mathbf{x} \in \partial D, \ \mathbf{\Omega} \cdot \mathbf{n} < 0. \tag{2.13}$$

Then, for all $\mathbf{x} \in D$ *and* $t > 0$,

$$B(\nu, T_L) \leqslant I(\mathbf{x}, \boldsymbol{\Omega}, \nu, t) \leqslant B(\nu, T_U), \tag{2.14}$$

$$T_L \leqslant T(\mathbf{x}, t) \leqslant T_U. \tag{2.15}$$

Thus, if a problem has initial and boundary data that lie between two Planckians, then the solution forever lies between these two Planckians. In this article, we show that numerical solutions obtained by the FC *algorithm must satisfy this maximum principle for sufficiently small time-steps, but not for sufficiently large time-steps.*

Equations (2.1) and (2.2) imply an energy conservation law which we now describe. Letting

$$E(\mathbf{x}, t) = \frac{1}{c} \iint I d\nu \, d\Omega \tag{2.16}$$

denote the radiative energy density, and

$$\mathbf{F}(\mathbf{x}, t) = \iint \boldsymbol{\Omega} I d\nu \, d\Omega \tag{2.17}$$

denote the radiative flux, we have from (2.1) and (2.2),

$$\frac{\partial}{\partial t}(\mathscr{E} + E) + \nabla \cdot \mathbf{F} = 0. \tag{2.18}$$

Integrating over D, we obtain

$$\frac{d}{dt} \int_D (\mathscr{E} + E) \, d^3x + \int_{\partial D} \mathbf{n} \cdot \mathbf{F} \, d^2x = 0, \tag{2.19}$$

which states that the time rate of change of the total material and radiative energy in D is equal to the net gain of radiative energy through ∂D. In this article we treat in detail a version of the FC method which exactly satisfies this conservation law.

III. The Fleck–Cummings Method

To describe the FC method, we define a sequence of times $0 = t_0 < t_1 < t_2 < \cdots$, with time steps $\Delta t_n = t_{n+1} - t_n$, and for $t_n \leqslant t \leqslant t_{n+1}$ we consider the following time-discretizations of (2.1) and (2.2)

$$\frac{1}{c} \frac{\partial I}{\partial t} + \boldsymbol{\Omega} \cdot \nabla I = \sigma_n \left(\frac{B_n}{\phi_n} \bar{\phi} - I \right), \tag{3.1}$$

$$\frac{\mathscr{E}(T_{n+1}) - \mathscr{E}(T_n)}{\Delta t_n} = \iint \sigma_n \left(I_{n+1/2} - \frac{B_n}{\phi_n} \bar{\phi}_{n+1/2} \right) d\nu \, d\Omega. \tag{3.2}$$

The boundary condition for (3.1) is given by (2.5), and the "initial" conditions for (3.1) and (3.2) are known from the previous time-step if $n>0$, or from (2.3) and (2.4) if $n=0$. Quantities in the above equations which are subscripted with an integer subscript n are evaluated at t_n, and quantities subscripted with $n+1/2$ are time-averaged over the nth time-step

$$I_{n+1/2}=\frac{1}{\Delta t_n}\int_{t_n}^{t_{n+1}} I\,dt, \tag{3.3}$$

$$\bar{\phi}_{n+1/2}=\frac{1}{\Delta t_n}\int_{t_n}^{t_{n+1}} \bar{\phi}\,dt. \tag{3.4}$$

Thus, the opacities in these equations are evaluated at the old time-step, and the emission term (Planck function) is approximated as

$$B[\nu, T(\mathbf{x}, t)]\approx\frac{B[\nu, T_n(\mathbf{x})]}{\phi_n(\mathbf{x})}\bar{\phi}(\mathbf{x}, t), \tag{3.5}$$

where $\bar{\phi}$ is to be determined. By (2.9) and (3.5), we have

$$\iint B[\nu, T(\mathbf{x}, t)]\,d\nu\,d\Omega\approx\bar{\phi}(\mathbf{x}, t), \tag{3.6}$$

and thus $\bar{\phi}(\mathbf{x}, t)$ physically approximates the equilibrium energy density.

Equations (3.1) and (3.2) are energy-conserving in the following sense: if we integrate (3.1) over $\mathbf{\Omega}$, ν, and $t_n<t<t_{n+1}$, add this to (3.2), and then integrate the resulting equation over $\mathbf{x}\in D$, we obtain the conservation law (2.19) integrated over $t_n<t<t_{n+1}$.

In order to solve (3.1)–(3.4), we must specify $\bar{\phi}$. To do this, we note that

$$\frac{\partial\mathscr{E}}{\partial t}=\frac{1}{\beta}\frac{\partial\phi}{\partial t}, \tag{3.7}$$

where

$$\frac{1}{\beta(T)}=\frac{d\mathscr{E}}{d\phi}=\frac{d\mathscr{E}}{dT}\left(\frac{d\phi}{dT}\right)^{-1}=\frac{c_v T}{4\phi}, \tag{3.8}$$

and we use this result to approximate (2.2) as

$$\frac{\hat{\phi}_{n+1}-\phi_n}{\beta_n\Delta t_n}=\iint\sigma_n\left(I_{n+1/2}-\frac{B_n}{\phi_n}\bar{\phi}_{n+1/2}\right)d\nu\,d\Omega, \tag{3.9}$$

$$\bar{\phi}_{n+1/2}=\alpha\hat{\phi}_{n+1}+(1-\alpha)\,\phi_n. \tag{3.10}$$

Here α is an arbitrary constant satisfying

$$\tfrac{1}{2}\leqslant\alpha\leqslant 1, \tag{3.11}$$

and we use the symbol $\hat{\phi}_{n+1}$ to emphasize that this quantity is not equal to $\phi_{n+1} = acT_{n+1}^4$. Eliminating $\hat{\phi}_{n+1}$ between (3.9) and (3.10), we obtain

$$\frac{\tilde{\phi}_{n+1/2}}{\phi_n} = \frac{\phi_n + \alpha\beta_n \Delta t_n \iint \sigma_n I_{n+1/2}\, dv\, d\Omega}{\phi_n + \alpha\beta_n \Delta t_n \iint \sigma_n B_n\, dv\, d\Omega}. \tag{3.12}$$

Consistent with (3.4), we define $\tilde{\phi}$ as

$$\frac{\tilde{\phi}}{\phi_n} = \frac{\phi_n + \alpha\beta_n \Delta t_n \iint \sigma_n I dv\, d\Omega}{\phi_n + \alpha\beta_n \Delta t_n \iint \sigma_n B_n\, dv\, d\Omega}. \tag{3.13}$$

Now we introduce (3.13) into (3.1), and (3.12) into (3.2). We obtain, after some straightforward algebra, the underlying equations for the FC method

$$\frac{1}{c}\frac{\partial I}{\partial t} + \boldsymbol{\Omega}\cdot\nabla I + \sigma_n I = \chi_n(1-f_n)\iint \sigma_n I dv'\, d\Omega' + \sigma_n f_n B_n, \quad t_n < t < t_{n+1}, \tag{3.14}$$

$$\mathscr{E}(T_{n+1}) = \mathscr{E}(T_n) + \Delta t_n f_n \iint \sigma_n (I_{n+1/2} - B_n)\, dv\, d\Omega, \tag{3.15}$$

where

$$\chi_n(\mathbf{x}, \nu) = \frac{\sigma_n B_n}{4\pi \int \sigma_n B_n\, dv}, \tag{3.16}$$

$$f_n(\mathbf{x}) = \frac{1}{1 + \alpha\beta_n \Delta t_n \sigma_{p,n}}, \tag{3.17}$$

$$\sigma_{p,n}(\mathbf{x}) = \frac{4\pi \int \sigma_n B_n\, dv}{\phi_n}. \tag{3.18}$$

Operationally, we now solve (3.14), with the previously described "initial" and boundary data, using a standard neutronics-based Monte Carlo algorithm [6, 7] or one with special modifications [8]. The exact solution of Eq. (3.14) exists, is unique, and is positive under very weak constraints on σ [9]. Then we compute $I_{n+1/2}$ from (3.3) and T_{n+1} from (3.15). Since $d\mathscr{E}/dT > 0$, this last step can be done uniquely, provided the right side of (3.15) is in the range of $\mathscr{E}$.

IV. Maximum Principle for the Fleck–Cummings Method

For $T_L < T_U$, let us define

$$\xi_1 = \sup_{T_L < T < T_U} \frac{16\pi\alpha}{c_v(T)} \int \sigma(\nu, T) \left[\frac{B(\nu, T_U) - B(\nu, T)}{T_U - T} - \frac{B(\nu, T)}{T} \right] d\nu \tag{4.1}$$

and

$$\xi_2 = \sup_{T_L < T < T_U} [\rho(T) - \alpha\beta(T)\,\sigma_p(T)], \tag{4.2}$$

where β is defined by (3.8), and ρ by

$$\rho(T) = \max\left\{\iint \sigma(\nu, T)\frac{B(\nu, T_U) - B(\nu, T)}{\mathscr{E}(T_U) - \mathscr{E}(T)}\,d\nu\,d\Omega,\right.$$
$$\left.\iint \sigma(\nu, T)\frac{B(\nu, T) - B(\nu, T_L)}{\mathscr{E}(T) - \mathscr{E}(T_L)}\,d\nu\,d\Omega\right\}. \tag{4.3}$$

Equation (2.8) and $0 < T < T_U$ imply

$$\frac{B(\nu, T_U) - B(\nu, T)}{T_U - T} - \frac{B(\nu, T) - B(\nu, 0)}{T - 0} > 0, \tag{4.4}$$

and since $B(\nu, 0) = 0$, we then have $\xi_1 > 0$. (However, ξ_2 need not be positive.) Rearranging (4.4), we get for all $0 < T \leqslant T_U$ and $0 < \nu < \infty$,

$$\frac{B(\nu, T_U)}{B(\nu, T)} > \frac{T_U}{T}. \tag{4.5}$$

We can now prove our main result

MAXIMUM PRINCIPLE. Let $0 \leqslant T_L < T_U$ be fixed constants, and let I_i, T_i, and I_b satisfy (2.11) through (2.13). Also, for every n, let

$$\Delta t_n[\max(\xi_1, \xi_2)] \leqslant 1. \tag{4.6}$$

Then, if I and T_n denote the FC specific intensity and material temperature, we have for all $t \geqslant 0$,

$$B(\nu, T_L) \leqslant I(\mathbf{x}, \boldsymbol{\Omega}, \nu, t) \leqslant B(\nu, T_U), \tag{4.7}$$

and for all integers $n \geqslant 0$

$$T_L \leqslant T_n(\mathbf{x}) \leqslant T_U. \tag{4.8}$$

Proof. The proof is by induction on the time step n. The induction hypothesis is that, for the nth time-step, if I_n and T_n satisfy (2.11) and (2.12) [this is true for $n = 0$], and if I_b satisfies (2.13) and Δt_n satisfies (4.6) [these are true for all n by assumption], then

$$B(\nu, T_L) \leqslant I(\mathbf{x}, \boldsymbol{\Omega}, \nu, t) \leqslant B(\nu, T_U), \qquad t_n \leqslant t \leqslant t_{n+1}, \tag{4.9}$$

and

$$T_L \leqslant T_{n+1}(\mathbf{x}) \leqslant T_U. \tag{4.10}$$

First we prove (4.9). To do this, we define

$$\psi(\mathbf{x}, \boldsymbol{\Omega}, \nu, t) = B(\nu, T_U) - I(\mathbf{x}, \Omega, \nu, t), \tag{4.11}$$

and we wish to show $\psi \geqslant 0$. Introducing $I = B_U - \psi$ into (3.14) and rearranging, we obtain

$$\frac{1}{c}\frac{\partial \psi}{\partial t} + \boldsymbol{\Omega} \cdot \nabla \psi + \sigma_n \psi - \chi_n(1 - f_n) \iint \sigma_n \psi \, d\nu' d\Omega' = Q, \tag{4.12}$$

$$Q(\mathbf{x}, \nu) = \sigma_n B_n \left[\left(\frac{B_U}{B_n} - 1 \right) - (1 - f_n) \frac{\int \sigma_n (B_U - B_n) \, d\nu'}{\int \sigma_n B_n \, d\nu'} \right], \tag{4.13}$$

where we have introduced $B_U = B(\nu, T_U)$ and $B_n = B(\nu, T_n)$.

By the induction hypothesis and (4.11), ψ has non-negative initial and boundary values. Thus, since ψ satisfies a standard linear transport problem, ψ is non-negative if the source term Q is non-negative [9]. Using the inequality (4.5) in (4.13), we get

$$Q \geqslant \sigma_n B_n \left[\left(\frac{T_U}{T_n} - 1 \right) - (1 - f_n) \frac{\int \sigma_n (B_U - B_n) \, d\nu'}{\int \sigma_n B_n \, d\nu'} \right], \tag{4.14}$$

which can be rearranged in the form

$$Q \geqslant \frac{\sigma_n B_n}{\int \sigma_n B_n \, d\nu'} (T_U - T_n) \left[\frac{1}{T_n} \int \sigma_n B_n \, d\nu' - \frac{1 - f_n}{T_U - T_n} \int \sigma_n (B_U - B_n) \, d\nu' \right]. \tag{4.15}$$

Using (3.17), we see that Q is non-negative if

$$\int \sigma_n \frac{B_n}{T_n} \, d\nu \geqslant \frac{\alpha \beta_n \, \Delta t_n \, \sigma_{p,n}}{1 + \alpha \beta_n \, \Delta t_n \sigma_{p,n}} \int \sigma_n \frac{B_U - B_n}{T_U - T_n} \, d\nu. \tag{4.16}$$

Rearranging, and using (3.8) and (3.18), we obtain the condition

$$\Delta t_n \left[\frac{16\pi\alpha}{c_{v,n}} \int \sigma_n \left(\frac{B_U - B_n}{T_U - T_n} - \frac{B_n}{T_n} \right) d\nu \right] \leqslant 1. \tag{4.17}$$

However, this is satisfied because, by assumption, $\Delta t_n \xi_1 \leqslant 1$. Hence $Q \geqslant 0$, which implies $\psi \geqslant 0$ and $I \leqslant B_U$.

In a similar manner, one can show that $B(\nu, T_L) = B_L \leqslant I$ if

$$\Delta t_n \left[\frac{16\pi\alpha}{c_{v,n}} \int \sigma_n \left(\frac{B_n - B_L}{T_n - T_L} - \frac{B_n}{T_n} \right) d\nu \right] \leqslant 1. \tag{4.18}$$

However, (2.8) implies, for $T_L < T_n < T_U$,

$$\frac{B_n - B_L}{T_n - T_L} < \frac{B_U - B_n}{T_U - T_n}. \tag{4.19}$$

Thus the integrand in (4.17) is larger than the integrand in (4.18) and, therefore, (4.18) is satisfied because (4.17) is. This completes the proof of (4.9), which gives

$$B(\nu, T_L) \leqslant I_{n+1/2}(\mathbf{x}, \Omega, \nu) \leqslant B(\nu, T_U). \tag{4.20}$$

Now, to prove (4.10), we shall instead verify the equivalent inequalities

$$\mathscr{E}(T_L) \leqslant \mathscr{E}(T_{n+1}) \leqslant \mathscr{E}(T_U). \tag{4.21}$$

Using (3.15) to eliminate $\mathscr{E}(T_{n+1})$, we obtain

$$\Delta t_n f_n \iint \sigma_n (I_{n+1/2} - B_n)\, d\nu\, d\Omega \leqslant \mathscr{E}(T_U) - \mathscr{E}(T_n), \tag{4.22a}$$

$$\Delta t_n f_n \iint \sigma_n (B_n - I_{n+1/2})\, d\nu\, d\Omega \leqslant \mathscr{E}(T_n) - \mathscr{E}(T_L). \tag{4.22b}$$

Using (4.20), we find that (4.22) are satisfied if

$$\Delta t_n f_n \iint \sigma_n \frac{B_U - B_n}{\mathscr{E}(T_U) - \mathscr{E}(T_n)}\, d\nu\, d\Omega \leqslant 1, \tag{4.23a}$$

$$\Delta t_n f_n \iint \sigma_n \frac{B_n - B_L}{\mathscr{E}(T_n) - \mathscr{E}(T_L)}\, d\nu\, d\Omega \leqslant 1. \tag{4.23b}$$

Introducing the definition (4.3) of ρ, we find that these inequalities are satisfied if and only if

$$\Delta t_n f_n \rho(T_n) \leqslant 1. \tag{4.24}$$

Finally, introducing the definition (3.17) of f_n and rearranging, we obtain the condition

$$\Delta t_n [\rho(T_n) - \alpha\beta_n \sigma_{p,n}] \leqslant 1, \tag{4.25}$$

which is satisfied because $\Delta t_n \xi_2 \leqslant 1$. This completes the proof of the inequalities (4.10), and also of the induction hypothesis. Therefore, the maximum principle is proved.

We note that the condition (4.6) gives sufficient conditions for the maximum principle to hold, but not necessary ones. In particular, if (4.6) is violated, then Q in Eq. (4.12) can (but need not) be negative for some values of its arguments. Also, if

Q has negative values, then ψ can (but need not) be negative for some values of its arguments. Moreover, for all Δt we have from (4.13)

$$\int Q dv = f_n \int \sigma_n (B_U - B_n)\, dv \geqslant 0, \tag{4.26}$$

and thus, even if Q has negative values, its frequency integral is always non-negative. For these reasons, it seems likely that the condition (4.6) is conservative, and that it will have to be substantially violated to obtain a solution which violates the maximum principle. We shall demonstrate this below in Section 6.

V. Maximum Principles for Related Methods

For an ideal gas, we have

$$\mathscr{E}(T) = c_v T, \tag{5.1}$$

where c_v is a constant. Also, for some applications, $\mathscr{E}(T)$ is nearly a linear function of T, so that $\mathscr{E}'(T) = c_v(T)$ is nearly constant. In such situations, one has

$$\mathscr{E}(T_{n+1}) - \mathscr{E}(T_n) \approx c_{v,n}(T_{n+1} - T_n), \tag{5.2}$$

and thus one can replace (3.15) by

$$T_{n+1} = T_n + \frac{\Delta t_n f_n}{c_{v,n}} \iint \sigma_n (I_{n+1/2} - B_n)\, dv\, d\Omega. \tag{5.3}$$

The resulting method does not strictly satisfy energy conservation, but it is simpler because (5.3) gives T_{n+1} directly, whereas (3.15) must be solved for T_{n+1}. This method also has a maximum principle, just like the one derived in Section 4, provided Δt_n satisfies

$$\Delta t_n \xi_1 \leqslant 1, \tag{5.4}$$

where ξ_1 is defined by (4.1). The analysis which leads to this result is very similar to that presented in Section 4, and will not be given here.

For the case of a "grey" problem, σ is independent of ν, and (2.1) can be integrated over ν to yield

$$\frac{1}{c}\frac{\partial \bar{I}}{\partial t} + \boldsymbol{\Omega} \cdot \nabla \bar{I} = \sigma(\bar{B} - \bar{I}), \tag{5.5}$$

$$\frac{\partial \mathscr{E}}{\partial t} = \sigma \int (\bar{I} - \bar{B})\, d\Omega', \tag{5.6}$$

where

$$\bar{I}(\mathbf{x}, \mathbf{\Omega}, t) = \int I(\mathbf{x}, \mathbf{\Omega}, v, t)\, dv, \tag{5.7}$$

$$\bar{B}(T) = \int B(v, T)\, dv = \frac{acT^4}{4\pi}. \tag{5.8}$$

Likewise, integrating (3.14) over v, we obtain for the FC equations

$$\frac{1}{c}\frac{\partial \bar{I}}{\partial t} + \mathbf{\Omega}\cdot\nabla\bar{I} + \sigma_n \bar{I} = \sigma_n\left[(1-f_n)\frac{1}{4\pi}\int \bar{I}\, d\Omega' + f_n \bar{B}_n\right], \tag{5.9}$$

$$\mathscr{E}(T_{n+1}) = \mathscr{E}(T_n) + \Delta t_n f_n \sigma_n \int (\bar{I}_{n+1/2} - \bar{B}_n)\, d\Omega. \tag{5.10}$$

One can now integrate (4.7) over v and obtain a maximum principle for $\bar{I}$ and T, with the required bound on Δt_n being given by (4.6), and ξ_1, ξ_2 defined by (4.1)–(4.3). However, these bounds were derived by using the inequality (4.5), which is relatively crude and does not lead to the weakest possible bound in the grey case. It happens that by deriving a maximum principle directly from (5.5)–(5.8), we obtain the best (weakest) rigorous bound

$$\Delta t_n \left\{ \sup_{T_L < T < T_U} \sigma(T)[\gamma(T) - \alpha\beta(T)] \right\} \leqslant 1, \tag{5.11}$$

$$\gamma(T) = \text{ac} \max\left[\frac{T_U^4 - T^4}{\mathscr{E}(T_U) - \mathscr{E}(T)}, \frac{T^4 - T_L^4}{\mathscr{E}(T) - \mathscr{E}(T_L)}\right]. \tag{5.12}$$

If (5.10) is replaced by

$$T_{n+1} = T_n + \frac{\Delta t_n f_n \sigma_n}{c_{v,n}} \int (\bar{I}_{n+1/2} - \bar{B}_n)\, dv, \tag{5.13}$$

then the bound on Δt_n which assures the maximum principle is

$$\Delta t_n \left\{ \text{ac} \sup_{T_L < T < T_U} \frac{\sigma(T)}{c_v(T)} \left[\frac{T_U^4 - T^4}{T_U - T} - 4\alpha T^3\right] \right\} \leqslant 1. \tag{5.14}$$

VI. Numerical Results and Discussion

We consider a slight variation of a problem discussed by Fleck and Cummings [3]. In our problem, a 4.0 cm slab with opacity

$$\sigma(v, T) = \gamma_0 \left(\frac{k}{hv}\right)^3 (1 - e^{-hv/kT}), \tag{6.1}$$

material energy

$$\mathscr{E}(T) = (\gamma_1 a T_0^3)\, T, \tag{6.2}$$

and initial temperature

$$T_i = 0.001 \text{ keV} \tag{6.3}$$

is heated on the left by a Planckian source with temperature

$$T_0 = 1.0 \text{ keV} \tag{6.4}$$

and on the right by a Planckian source with temperature T_i. The constants in this problem are

$$\gamma_0 = 27 \text{ keV}^3/\text{cm}, \tag{6.5a}$$

$$\gamma_1 = 0.5917, \tag{6.5b}$$

and we consider the multifrequency algorithm described in Section 5 with $\alpha = 1$. (This algorithm is identical to the one described in Sect. 4 because $\mathscr{E}$ is linear in T.)

The FC solution of this problem must satisfy the maximum principle, with $T_L = T_i$ and $T_U = T_0$, provided Δt satisfies the bound (5.4). Using (6.1) and (6.2), and omitting much straightforward algebra, one can reformulate this bound as

$$\Delta t \leqslant \frac{T_0^3 \gamma_1 \gamma_2}{\gamma_0 F(T_L/T_U)}, \tag{6.6}$$

where

$$F(r) = \sum_{n=1}^{\infty} \frac{1}{(1+n)(1+rn)}, \qquad 0 < r \leqslant 1, \tag{6.7}$$

and

$$\gamma_2 = 5.411 \times 10^{-11} \text{ sec/cm}.$$

The function $F(r)$ is plotted in Fig. 1. It decreases monotonically from $F(0) = \infty$ to $F(1) = \pi^2/6 - 1 = 0.645$ as r increases from 0 to 1. Using $F(0.001) = 6.492$, Eq. (6.6) yields

$$\Delta t \leqslant 1.827 \times 10^{-13} \text{ sec} \tag{6.8}$$

as the theoretical bound on Δt which guarantees that the solution will satisfy the maximum principle.

This problem differs from the original Fleck–Cummings problem [3] only in that in [3], there is no source of photons on the right edge of the slab. This "vacuum" boundary condition corresponds to a Planckian with zero temperature; therefore,

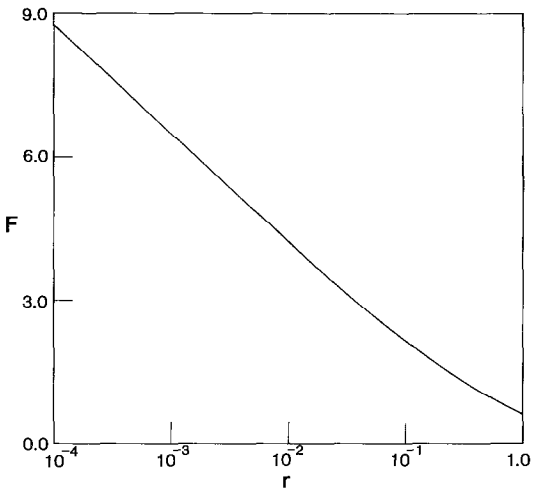

FIG. 1. The function $F(r)$.

the exact solution of this problem satisfies the maximum principle with $T_U = 1.0$ keV and $T_L = 0.0$ keV. However, since $F(0) = \infty$, the bound (6.6) gives $\Delta t = 0$, and thus our theory does not guarantee a Monte Carlo solution satisfying the maximum principle for any positive time-step. Nevertheless, our calculations indicate that the FC solution does satisfy the maximum principle, roughly for

$$\Delta t \leqslant 7.4 \times 10^{-11} \text{ sec.} \tag{6.9}$$

In [3], Fig. 4 clearly displays a violation of the maximum principle for $\Delta t = 2 \times 10^{-10}$ sec, but not in Fig. 3 for $\Delta t = 10^{-10}$ sec. However, the Fig. 3 plot is for $t = 2 \times 10^{-10}$ sec, hence is the result after two time-steps. For $\Delta t = 10^{-10}$ sec, our calculations show a violation of the maximum principle only at the end of the first time-step, and hence this violation is not visible at later times.

In Fig. 2, we plot the material temperature for our problem across the slab at the end of one time step, with $\Delta t = 2 \times 10^{-10}$ sec. As in [3], we divide the slab into 10 equal spatial cells, and cell-average temperatures are plotted at cell centers and are joined by straight lines. Since the difference between our problem and the problem in [3] is small, our result agrees fairly well with that shown in Fig. 4 in [3], and the violation of the maximum principle in the leftmost cell is apparent. This violation disappears in our problem for Δt roughly satisfying (6.9). This numerically observed bound is considerably larger than the theoretical bound (6.8).

These results indicate that our general theoretical bound (4.6) is very conservative. That is, the smallest value of Δt for which the FC solution will violate the maximum principle can be much larger than the theoretical bound which guarantees that the maximum principle will not be violated.

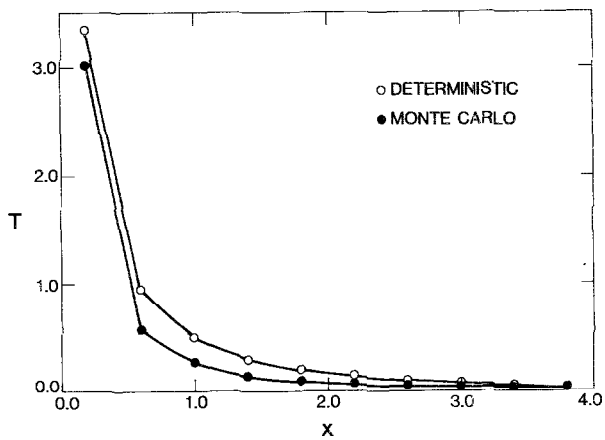

FIG. 2. Material temperatures for $t = \Delta t = 2 \times 10^{-10}$ sec.

We now discuss, with little detail, some additional results which we have observed in our numerical experimentation. In particular, we have run our problem for longer times, using the "pure" FC algorithm described above, also using the random walk approximation to speed up the numerical calculations [8], and additionally, using a deterministic method very similar to that described in [4] and based directly on the multifrequency method described above in Section 5. In all cases we observed very similar behavior. For $\Delta t = 2 \times 10^{-10}$ sec, the solutions violate the maximum principle in the leftmost cell, but after a few time-steps this inaccuracy disappears and the solutions then converge to the correct steady-state solution. (The material temperatures are plotted in Fig. 2 for the two Monte Carlo methods, which agree to within 0.05 keV, and the deterministic method.) As the time step is increased, the solutions after one time-step increase in the leftmost cell, the violation of the maximum principle can extend to two or more cells, and an increasingly large number of time steps is required for this inaccuracy to disappear and the solutions to converge to the steady-state solution. For every Δt which we selected, the solutions did eventually converge to the correct steady-state solution; thus, in this sense, the method is stable.

Finally, in some further experimentation on our problem, we found, in general, that for any fixed Δt and $T_i \neq T_0$, we could always make the solutions violate the maximum principle after one time-step by taking the opacity multiplier γ_0 large enough.

We now summarize our analytical and numerically-observed results.

(i) The ideal FC solution must satisfy the maximum principle for a small enough time-step and opacity multiplier, but it can, and generally does, violate the maximum principle for a large enough time-step or opacity multiplier.

(ii) The theoretical bound (4.6) on Δt, which guarantees that the FC solution

satisfies the maximum principle, is much smaller than the actual value of Δt at which the violation of the maximum principle occurs. Thus, although this theoretical bound is correct, it is very conservative and not likely to be useful in predicting how large a time step can be chosen before the maximum principle is violated.

(iii) The violation of the maximum principle occurs in pure Monte Carlo, Monte Carlo with random walk, and deterministic solutions which are obtained using, as a basis, the algorithm described in Section 3. These violations occur because of properties of the underlying equations in Section 3, not because of the use of an inadequate number of particles in the Monte Carlo methods, or an inadequate differencing scheme in the deterministic methods.

(iv) The FC algorithm appears to be stable, in the sense that for every finite Δt, the FC solution of our problem remains bounded and approaches the correct steady-state solution as $t \to \infty$. However, for large and increasing Δt, the transient part of the solution becomes increasingly unphysical for increasingly many time-steps.

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