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THE CALCULATION OF NONLINEAR RADIATION TRANSPORT
BY A MONTE CARLO METHOD

(Title: Unclassified)

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November 13, 1961

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The Calculation of Nonlinear Radiation Transport

By A Monte Carlo Method

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ABSTRACT

A Monte Carlo method of solving the one-dimensional equations of nonlinear radiation transport is compared with the S_n "characteristics" method of solution. It is concluded that the Monte Carlo method is accurate and stable and furthermore for a given time-cycle length and space-zone size the Monte Carlo method is more accurate than the S_n method.

The Calculation of Nonlinear Radiation Transport

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I. INTRODUCTION

The areas of application of the Monte Carlo method in physics are numerous. In nearly all cases the technique is applied under conditions which may be regarded as linear. One area of frequent application is neutron transport. The transport of particles in this case may be assumed to depend on the geometry of the system in question, the scattering and absorbing properties of the media which it contains, but to be independent of the particle densities. The transport equation which describes this phenomenon is of course linear. The transport of dense gases on the other hand involves collisions between the gas molecules themselves and gives rise to a nonlinear problem. Further examples of nonlinear transport phenomena are found in the field of radiative transfer. Since the transport of radiation through a medium affects its absorption properties, the transport of individual photons is indirectly affected by the density of the other photons present. The resulting problem is therefore nonlinear.

In the usual applications of the Monte Carlo technique to linear transport problems, one or more quantities pertaining to a given system are computed for each of a reasonably large number of independent particle histories. The desired numbers are obtained by averaging the results over all of the histories. In the case of nonlinear transport phenomena, the motion of individual particles is influenced by the motion of all of the other particles. One cannot, therefore, calculate the behavior of the system simply by taking averages over independent particle histories.

One possible approach to the solution of nonlinear transport problems is to set up a model containing a reasonably large number of mutually interacting particles and to determine their trajectories by simultaneously solving their equations of motion. Alder and Wainwright (1957) have applied this method to problems relating to the theory of liquids. Following a large system of correlated particles can, however, be vastly more complicated and time-consuming than following an equivalent number of uncorrelated particles.

In the transport of radiation there exists a single parameter, temperature, which completely characterizes the nonlinearity of the problem. This simplifies the problem and suggests the following scheme for its solution. From the initial temperature distribution a source distribution is constructed and a population of independent photons generated. These photons are followed and periodically examined. The results of these examinations determine new temperature and source distributions from which new photons are generated. The continual absorption of photons limits the number of particles that must be followed at any time. The calculation is time dependent, but steady-state solutions which are of interest in astrophysical applications may be obtained by considering the solutions at large time.

II. DESCRIPTION OF THE PROBLEM

The equations that govern the transport of radiation through matter in one dimension are the transport equation,

$$\frac{1}{c} \frac{\partial I_\nu}{\partial t} + \mu \frac{\partial I_\nu}{\partial x} = \kappa' \rho (2\pi B_\nu(T) - I_\nu) - \sigma_s \rho \int_0^{2\pi} d\phi \int_{-1}^1 p(\cos \Theta) I_\nu(x, t, \mu') d\mu', \quad (1)$$

and the equation of energy conservation,

$$\rho c_v \frac{\partial T}{\partial t} = -2\tau \int_0^\infty \kappa_\nu I_\nu d\nu + \int_{-1}^1 d\mu \int_0^\infty \kappa_\nu \rho I_\nu d\nu. \quad (2)$$

In these equations $I_\nu(x, t, \mu)$ is the radiation intensity at position x , time t , and in direction μ , per unit value of μ . The quantity μ is the cosine of the angle between the direction in question and the x axis. See Fig. 1. The intensity I_ν , it will be noted, is 2π times the intensity per unit solid angle. The following relations also hold for the intensity I_ν :

$$J_\nu(x, t) = \frac{1}{2} \int_{-1}^1 I_\nu(x, t, \mu) d\mu \quad (3a)$$

$$u(x, t) = \frac{1}{c} \int_0^\infty d\nu \int_{-1}^1 I_\nu(x, t, \mu) d\mu, \quad (3b)$$

where $J_\nu(x, t)$ is defined as the mean intensity, and $u(x, t)$ is the radiation energy density. The function $B_\nu(T)$ is the Planck function at temperature T :

$$B_\nu(T) = \frac{2h\nu^3}{c^2} \frac{1}{e^{h\nu/kt} - 1}. \quad (4)$$

σ_s is the radiation scattering cross section, and c_v is the specific heat of the medium. The mass absorption coefficient κ_ν' is obtained from the "true" mass absorption coefficient κ_ν by correcting for induced emission:

$$\kappa_\nu' = (1 - e^{-h\nu/kt}) \kappa_\nu. \quad (5)$$

The function $p(\cos \theta)$ is the phase function which gives the distribution of $\cos \theta$, where θ is the angle of scattering of the light quanta. For Thomson scattering of light quanta by electrons, the phase function is

$$p(\Theta) = \frac{3}{16\pi} (1 + \cos^2 \Theta). \quad (6)$$

The quantity $\cos \Theta$ can be expressed as

$$\cos \Theta = \mu\mu' + (1 - \mu^2)^{1/2} (1 - \mu'^2)^{1/2} \cos(\phi - \phi'), \quad (7)$$

where μ and μ' are the values of μ and μ' before and after the collision, and ϕ and ϕ' are the values of the azimuthal angle made by the photon directions before and after the collision. If expression (6) is substituted into Eq. (1), the result is

$$\frac{1}{c} \frac{\partial I_\nu}{\partial t} + \mu \frac{\partial I_\nu}{\partial x} = \kappa_\nu' \rho (2\pi B_\nu(T) - I_\nu) - \sigma_s I_\nu + \frac{3}{16} \sigma_s \left[(3 - \mu^2) \int_{-1}^1 I_\nu(\mu') d\mu' + (3\mu^2 - 1) \int_{-1}^1 I_\nu(\mu') \mu'^2 d\mu' \right]. \quad (8)$$

Equation (8) applies to the frequency-dependent or nongrey case. We wish for the present to restrict our attention to the grey case, considering only the intensity I which has been integrated over frequency:

$$I = \int_0^\infty I_\nu d\nu. \quad (9)$$

This requires that we find some suitable average for the absorption coefficient κ_ν' . Without attempting further justification we assume that

$$\kappa = \frac{\int_0^\infty \kappa_\nu B_\nu(T) d\nu}{\int_0^\infty B_\nu d\nu} \quad (10)$$

The resulting integrated forms of Eqs. (1) and (2) are

$$\frac{1}{c} \frac{\partial I}{\partial t} + \mu \frac{\partial I}{\partial x} = \kappa \rho \left(\frac{caT^4}{2} - I \right) - \sigma_s I + \frac{3}{16} \sigma_s \left[(3 - \mu^2) \int_{-1}^1 I(\mu') d\mu' + (3\mu^2 - 1) \int_{-1}^1 I(\mu') \mu'^2 d\mu' \right], \quad (11)$$

$$\rho c_v \frac{\partial T}{\partial t} = - \kappa \rho (caT^4 - \int_{-1}^1 I d\mu). \quad (12)$$

In developing a Monte Carlo method of solution for Eqs. (11) and (12), rather than for the Eqs. (1) and (2) which apply to the frequency-dependent case, there is actually no important loss in generality. In generalizing the method to the nongrey case one need only consider photons which are sampled from a source distribution depending on frequency as well as on position.

The specific problem which we shall consider is the irradiation of a slab of finite thickness, extending from $x = 0$ to $x = L$, by a hohlraum held at a fixed temperature $T = T_0$ and situated at $x = 0$. See Fig. 1.

III. FINITE DIFFERENCE METHODS OF SOLUTION

The more conventional method of solving Eqs. (11) and (12) involves reducing them to finite difference form or to a combination of finite difference and semianalytic form. A certain amount of discussion will be devoted to this approach since it suggests how the Monte Carlo technique can be applied to the problem and since it also furnishes numerical solutions which can be compared with the Monte Carlo solutions.

Let us define M discrete values of μ by

$$\mu_m = -1 + \frac{2m-1}{M}, \quad m = 1, 2, \dots, M \quad (13)$$

and the corresponding fluxes by

$$I_m(x, t) = I(\mu_m, x, t). \quad (14)$$

Equations (11) and (12) may now be approximated by

$$\frac{1}{c} \frac{\partial I_m}{\partial t} + \mu_m \frac{\partial I_m}{\partial x} = \kappa \rho \left(\frac{c a T^4}{2} - I_m \right) - \sigma_s I_m + \frac{3}{10} \sigma_s \left[\left(3 - \mu_m^2 \right) \frac{2}{M} \sum_{m=1}^M I_m + \left(3\mu_m^2 - 1 \right) \frac{2}{M} \sum_{m=1}^M I_m \mu_m^2 \right], \quad (15)$$

$$\rho c_v \frac{\partial T}{\partial t} = - \kappa \rho \left(c a T^4 - \frac{2}{M} \sum_{m=1}^M I_m \right). \quad (16)$$

Equations (14)-(16) represent a form of discrete flux approximation to Eqs. (11) and (12). A steady-state solution to another discrete flux approximation of these equations was first obtained by Wick (1943) and Chandrasekhar (1950). In their method the directions μ_m were chosen so that the integral over intensity could be approximated by the Gauss quadrature formula. The discrete directions in Eq. (14) have been selected only for reasons of convenience. This choice of directions has also been employed by Carlson (1959) in a method of neutron transport calculation known as the DS_n method.

Equations (14) and (15) can be further approximated in finite difference form and solved. This method has been used by Barfield (1954) et al. One could also solve Eq. (16) by a finite difference approximation and solve the system of hyperbolic equations (15) in a semianalytic form by integrating along characteristics. The latter method was first suggested by Keller and Wendroff (1956), although no numerical results of the method have been published. The "characteristics" S_n method has been selected for numerical comparison with the Monte Carlo method. It will be referred to in the

Fig. 1

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Fig. 2

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remainder of this article as simply the "S₁" method. A brief description of the method is now presented.

Consider the slab divided into regions bounded by the planes $x = x_j = j \Delta x$, $j = 0, 1, \dots, J$, $J \Delta x = L$. Consider also the time divided into intervals of duration Δt . Thus a two-dimensional mesh in space and time may be constructed (see Fig. 2). The differential operator on the left-hand side of Eqs. (15) may be replaced by a directional derivative,

$$\frac{1}{c} \frac{\partial}{\partial t} + \mu_m \frac{\partial}{\partial x} = D_m \frac{d}{ds}, \quad (17)$$

where d/ds signifies differentiation along a line whose direction cosines with the x and t axes are, respectively,

$$1/c D_m, \mu_m/D_m, \quad (18)$$

where

$$D_m = \left[(1/c^2) + \mu_m^2 \right]^{1/2}. \quad (19)$$

Equations (15) may now be written

$$D_m \frac{dI_m}{ds} + (\kappa_p + \sigma_s) I_m = S_m, \quad m = 1, 2, \dots, M \quad (20)$$

where S_m is the sum of the temperature-dependent source and the scattered particle source. The solution to Eqs. (19) at a mesh point Q in terms of values of I_m and S_m at an earlier time but not necessarily at a mesh point is

$$I_{mQ} = I_{mP} e^{-\frac{1}{D_m} \int_0^s (\kappa_p + \sigma) ds} + \frac{1}{D_m} \int_0^s S_m(s') e^{-\frac{1}{D_m} \int_{s'}^s (\kappa_p + \sigma_s) ds''} ds'. \quad (21)$$

In Eq. (21) and in what follows the points P and Q refer to Fig. 2. If we approximate the source function by

$$S_m \approx \frac{1}{2}(S_P + S_Q) \quad (22)$$

and regard the temperature in a given mesh rectangle as a constant equal to its value at the center of the rectangle, i. e. ,

$$T = T \left[\left(n + \frac{1}{2} \right) \Delta t, x_j \pm \Delta x/2 \right] = T_{j \pm \frac{1}{2}}^{n + \frac{1}{2}}, \quad (23)$$

then Eq. (20) can be approximated as

$$I_{mQ} = I_{mP} e^{-\sigma_{j \pm \frac{1}{2}}^{n + \frac{1}{2}} \Delta s / D_m} + \frac{S_P + S_Q}{2\sigma_{j \pm \frac{1}{2}}^{n + \frac{1}{2}}} \left(1 - e^{-\sigma_{j \pm \frac{1}{2}}^{n + \frac{1}{2}} \Delta s / D_m} \right). \quad (24)$$

In Eqs. (23) and (24) the plus and minus signs correspond to the cases where the characteristic has negative and positive slopes, respectively.

Also

$$\sigma_{j \pm \frac{1}{2}}^{n + \frac{1}{2}} = \kappa_{j \pm \frac{1}{2}}^{n + \frac{1}{2}} \rho + \sigma_s, \quad (25)$$

and Δs is the length of the line segment PQ. The quantities I_{mP} and S_P are determined by linear interpolation from values of I_m and S expressed at mesh points. In this computation two cases must be distinguished:

Case I: $c \Delta t |\mu_m| < \Delta x$

$$I_{mQ} = I_{mP} e^{-\sigma_{j \pm \frac{1}{2}}^{n + \frac{1}{2}} c \Delta t} + \frac{S_P + S_Q}{2\sigma_{j \pm \frac{1}{2}}^{n + \frac{1}{2}}} \left(1 - e^{-\sigma_{j \pm \frac{1}{2}}^{n + \frac{1}{2}} c \Delta t} \right) \quad (26)$$

$$I_{mP} = \frac{1 - c \Delta t \mu_m}{x_j - x_{j\pm 1}} I_{mQ} + \frac{c \Delta t \mu_m}{x_j - x_{j\pm 1}} I_{mQ_0} \quad (27)$$

$$S_{mP} = \frac{1 - c \Delta t \mu_m}{x_j - x_{j\pm 1}} S_{mQ} + \frac{c \Delta t \mu_m}{x_j - x_{j\pm 1}} S_{mQ_0} \quad (28)$$

Case II: $c \Delta t |\mu_m| > \Delta x$

$$I_{mQ} = I_{mP} e^{-\sigma_{j\pm\frac{1}{2}}^{n+\frac{1}{2}} \Delta x / \mu_m} + \frac{S_P + S_Q}{2\sigma_{j\pm\frac{1}{2}}^{n+\frac{1}{2}}} \left(1 - e^{-\sigma_{j\pm\frac{1}{2}}^{n+\frac{1}{2}} \Delta x / \mu_m} \right) \quad (29)$$

$$I_{mP} = \left[1 - \frac{x_j - x_{j\pm 1}}{c \Delta t \mu_m} \right] I_{mQ_1} + \frac{x_j - x_{j\pm 1}}{c \Delta t \mu_m} I_{mQ_0} \quad (30)$$

$$S_{mP} = \left[1 - \frac{x_j - x_{j\pm 1}}{c \Delta t \mu_m} \right] S_{mQ_1} + \frac{x_j - x_{j\pm 1}}{c \Delta t \mu_m} S_{mQ_0} \quad (31)$$

The order in which the solution proceeds is in the direction of increasing x for μ_m positive and in the direction of decreasing x for negative μ_m . The boundary conditions are

$$\begin{aligned} I_m(x=0) &= aT^4/2 & \mu_m > 0 \\ I_m(x=L) &= 0 & \mu_m < 0. \end{aligned} \quad (32)$$

In computing the scattering contribution to S_Q in Eqs. (24) to (29) it is necessary to know the values of I_m which it is desired to compute. An iterative procedure may be used whereby initially the scattering source is computed using values of I_m at time t^n . The values of I_m at time t^{n+1} are then computed and the scattering source at Q is improved.

In the calculation as described thus far it has been assumed that the radiation intensities I_m are calculated at times $t^n = n \Delta t$ and positions $x_j = j \Delta x$ and that the temperatures are calculated at times $t^{n \pm \frac{1}{2}} = (n \pm \frac{1}{2}) \Delta t$ and positions $x_{j \pm \frac{1}{2}} = (j \pm \frac{1}{2}) \Delta x$. One could equally well use Eqs. (26)-(32) to advance the radiation intensities I_m from time $t^{n-\frac{1}{2}}$ to time $t^{n+\frac{1}{2}}$ using values of temperature at time t^n to calculate absorption coefficients and source terms and then use the following difference equation derived from Eq. (16) to advance the temperature from time t^n to time t^{n+1} .

$$T_{j-\frac{1}{2}}^{n+1} = T_{j-\frac{1}{2}}^n - \frac{c \Delta t}{\rho c v} \kappa \left(T_{j-\frac{1}{2}}^{n+\frac{1}{2}} \right)^2 \left[\left(T_{j-\frac{1}{2}}^{n+\frac{1}{2}} \right)^4 - \frac{2}{M} \sum_{m=1}^M I_{mj-\frac{1}{2}}^{n+\frac{1}{2}} \right], \quad (33)$$

where

$$\begin{aligned} T_{j-\frac{1}{2}}^{n+\frac{1}{2}} &= \left(T_{j-\frac{1}{2}}^{n+1} + T_{j-\frac{1}{2}}^n \right) / 2 \\ I_{j-\frac{1}{2}}^{n+\frac{1}{2}} &= \left(I_{mj}^{n+\frac{1}{2}} + I_{mj-1}^{n+\frac{1}{2}} \right) / 2. \end{aligned} \quad (34)$$

Note that Eq. (33) is centered at $t = t^{n+\frac{1}{2}}$. The procedure can be started by assuming that the values of I_m at time $t = 0$ hold at $t^{-\frac{1}{2}}$.

IV. THE MONTE CARLO METHOD OF SOLUTION

We may summarize the calculation procedure just described as follows:

1. The transport equation is solved assuming a temperature distribution which is constant during a given time cycle and throughout a given spatial zone. In so doing the radiation intensities are advanced from time $t^{n-\frac{1}{2}}$ to time $t^{n+\frac{1}{2}}$.
2. The radiation intensities obtained from step 1 are used to calculate radiation absorption rates at time $t^{n+\frac{1}{2}}$ which in turn are substituted

into finite difference equations. The latter are used to advance the temperatures from time t^n to t^{n+1} . The entire cycle is then repeated using the new temperatures.

The essential feature of step 1 is that the calculation is performed under the assumption of temperature and medium properties constant in time. We could also have solved this part of the problem by a conventional Monte Carlo procedure. It would be required to generate photons or, more appropriately, energy bundles from a known temperature distribution. These "particles" would be followed in time and space while appropriate account is taken of absorption and scattering processes. At census time, i. e., at the end of a time cycle, the radiation energy is tallied in each zone. This in turn is used as the input to step 2 described above.

In the problem under discussion there will be two types of sources. The first type is the surface source:

$$S_0 = \sigma T_0^4, \quad (35)$$

where $\sigma = ac/4$ = Stephan's constant. The second type is the "volume" source:

$$S_{j-\frac{1}{2}}^n = 4\sigma \left(T_{j-\frac{1}{2}}^n \right)^4 \Delta x, \quad j=1, \dots, J. \quad (36)$$

Equations (35) and (36) describe the rates at which the surface $x = 0$ and the various zones of heated material radiate energy. Let N_1 be an input number which cannot be exceeded by the number of source particles generated in a given time cycle. Then the number of surface source particles N_0^n and the number $N_{j-\frac{1}{2}}^n$ of volume source particles generated in a given time cycle may be determined from the following equations:

$$N_0^n = \text{Grint} \left[\frac{T_0^4 N_1}{T_0^4 + 4\Delta x \sum_{j=1}^J \rho \kappa_{j-\frac{1}{2}}^n \left(\frac{T_0^n}{T_{j-\frac{1}{2}}^n} \right)^4} \right] \quad (37)$$

$$N_{j-\frac{1}{2}}^n = \text{Grint} \left[\frac{4\Delta x \sum_{j=1}^J \rho \kappa_{j-\frac{1}{2}}^n \left(\frac{T_0^n}{T_{j-\frac{1}{2}}^n} \right)^4 N_1}{T_0^4 + 4\Delta x \sum_{j=1}^J \rho \kappa_{j-\frac{1}{2}}^n \left(\frac{T_0^n}{T_{j-\frac{1}{2}}^n} \right)^4} \right]$$

In Eqs. (37) Grint signifies the greatest integer less than the argument. The energy of the various source particles is given by

$$E_0^n = \Delta t \sigma T_0^4 / N_0^n \quad (38)$$

$$E_{j-\frac{1}{2}}^n = \Delta t \Delta x 4\rho \kappa_{j-\frac{1}{2}}^n \left(\frac{T_0^n}{T_{j-\frac{1}{2}}^n} \right)^4 / N_{j-\frac{1}{2}}^n$$

The use of Eqs. (37) and (38) insures that energy is conserved and that the most particles are generated where the most energy is radiated. Since a nearly constant number of new particles is generated during each time cycle, the total number of particles being followed in a given time cycle will increase at first. A steady state, however, is eventually reached, and if the number N is judiciously chosen, the total number of particles reaching census in any specified time cycle can be kept within a specified bound determined by the storage capacity of the machine.

To be on the safe side one may use the following procedure with a varying N_1 . Let N be an upper bound to the number of particles which can be allowed to reach census, and let N_2 be the number of particles which reached census at the end of the previous time cycle. Then N_1 for the current time cycle may be chosen so that

$$N_1 + N_2 \leq N. \quad (39)$$

Once the energy, number, and location of the source particles has been decided, they are assigned starting position and time coordinates x_0 , t_0 as well as directions μ_0 . The two types of source particles are handled according to the following two schemes:

Surface particles:

$$x_0 = 0 + \delta \text{ (}\delta \text{ a small positive number)} \quad (40a)$$

$$t_0 = (n - 1/2 + r) \Delta t \quad (40b)$$

$$\mu_0 = \max (r_1, r_2) \quad (40c)$$

Volume particles, zone j ; $j = 1, 2, \dots, J$

$$x_0 = (j - 1 + r) \Delta x \quad (41a)$$

$$t_0 = (n - 1/2 + r) \Delta t \quad (41b)$$

$$\mu_0 = 2r - 1 \quad (41c)$$

In the above equations as well as in what follows r stands for a random number between 0 and 1. Since the particles in the hohlraum adjacent to the surface $x = 0$ are considered isotropic, the actual number crossing this surface from the hohlraum in a given direction will be weighted by the cosine of the angle which this direction makes with the x axis, i. e.,

$$f(\mu_0) = 2\mu_0, \quad (42)$$

where $f(\mu)$ is the distribution function of the direction μ_0 . (This is equivalent to the first of the boundary conditions expressed in Eq. (32).) The volume particles are emitted isotropically, i. e., uniformly distributed in μ .

Once the particle data are determined, the geometry routine is entered. The latter begins with the determination of the distance to boundary d_B , the distance to collision d_{col} , and the distance to census d_{cen} , where

$$d_B = \begin{cases} [(j+1)\Delta x - x]/\mu, & \text{if } \mu \geq 0 \\ (x - j\Delta x)/\mu, & \text{if } \mu < 0 \end{cases} \quad (43)$$

$$d_{col} = \lambda_{j-\frac{1}{2}}^n |\ln r| \quad (44)$$

$$\lambda_{j-\frac{1}{2}}^n = (\sigma_s + \kappa_{j-\frac{1}{2}}^n \rho)^{-1} \quad (45)$$

$$d_{cen} = c \left[(n+1) \Delta t - \epsilon \right] \quad (46)$$

Here x and t represent the position and time of the particle. The next step is determined by which of these distances is smallest. If the smallest distance d turns out to be d_{cen} , the particle is advanced in position and time:

$$\begin{aligned} x' &= x + \mu d \\ t' &= t + d/c \\ \mu' &= \mu, \end{aligned} \quad (47)$$

the particle data is stored, and the energy is tallied for the appropriate zone. If the smallest distance turns out to be d_B , the particle is advanced to

$$\begin{aligned} x' &= x + \mu d' \\ t' &= t + d'/c \\ d' &= d + \delta \quad (\delta \text{ a small number}), \end{aligned} \quad (48)$$

and the new zone number j of the particle is determined by

$$j = \text{Grint}(x'/\Delta x). \quad (49)$$

If $j \geq J$ the particle is lost from the system and the history is ended. Otherwise the calculation and selection using Eqs. (40)-(43) is repeated. However, after a boundary crossing, Eq. (44) may be replaced by

$$d_{\text{col}}^i = \frac{\lambda_{j-1/2}^{i-1/2}}{\lambda_{j-1/2}^i} (d_{\text{col}}^{i-1} - d_{\text{col}}^i), \quad (50)$$

where d_{col} and d_B are retained from the previous use of Eqs. (43)-(46).

In case $d = d_{\text{col}}$ is selected, the specific collision type must be determined. The process is absorption if

$$r \leq \kappa_{j-1/2}^n \rho / \left(\kappa_{j-1/2}^n \rho + \sigma_a \right) \quad (51)$$

and scattering otherwise. If the process is absorption, the history is terminated. If the process is scattering, the particle is first advanced:

$$\begin{aligned} x' &= x + \mu d \\ t' &= t + d/c, \end{aligned} \quad (52)$$

and a new direction is selected using the phase function for Thomson scattering (Eq. (6)). The phase function for Eq. (6), gives the distribution in the cosine of the scattered angle Θ per unit solid angle. If expression (7) for $\cos \Theta$ is substituted into the phase function, the following expression is obtained for the distribution in final direction per unit solid angle:

$$\begin{aligned} p(\mu, \mu', \phi, \phi') &= \frac{3}{16\pi} \left[1 + \mu^2 \mu'^2 + 2\mu\mu'(1-\mu^2)^{\frac{1}{2}}(1-\mu'^2)^{\frac{1}{2}} \cos(\phi - \phi') \right. \\ &\quad \left. - (1-\mu^2)(1-\mu'^2) \cos^2(\phi - \phi') \right]. \end{aligned} \quad (53)$$

If Eq. (43) is integrated over azimuth, i. e., over ϕ for fixed ϕ' , the result is

$$\begin{aligned} p(\mu, \mu') &= p(\mu', \mu) \\ &= \frac{3}{16} \left[(3 - \mu^2) + (3\mu^2 - 1) \mu'^2 \right], \end{aligned} \quad (54)$$

where $p(\mu, \mu')$ is the probability of scattering from μ to μ' per unit value of μ in $d\mu$. Note that

$$\int_{-1}^1 p(\mu, \mu') d\mu' = \int_{-1}^1 p(\mu', \mu) d\mu = 1. \quad (55)$$

Figure 3 shows the function $p(\mu, \mu')$ for three different values of μ . For a given μ the value of μ' can be determined by the following rejection technique:

Select r_1 and r_2

Case 1: $\mu^2 \leq 1/3$

Let $x = 2r_1 - 1$.

If $(3 - \mu^2) + (3\mu^2 - 1)x^2 \leq (3 - \mu^2)r_2$, $\mu' = x$.

Otherwise two new random numbers are selected and the procedure is repeated.

Case 2: $\mu^2 > 1/3$

Let $x = 2r_1 - 1$.

If $(3 - \mu^2) + (3\mu^2 - 1)x^2 \leq 2r_2(1 - \mu^2)$, $\mu' = x$.

Otherwise two new random numbers are selected and the procedure is repeated.

The residue particles, i. e., particles generated in previous time cycles which have reached census at time $t^{n-\frac{1}{2}}$, are treated in all respects like the source particles, except that their starting position and time coordinates as well as direction are those associated with the particle at the last census. Finally, the energy $E_{j-\frac{1}{2}}^{n+\frac{1}{2}}$ of all particles reaching census in a given zone is summed. From these sums the intensity integrated over angle in that zone is obtained.

$$\int_{-1}^1 I_{j-\frac{1}{2}}^{n+\frac{1}{2}} d\mu = c \sum E_{j-\frac{1}{2}}^{n+\frac{1}{2}} / \Delta x \quad (56)$$

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Fig. 3. The distribution $p(\mu, \mu')$ of the scattered photon direction.

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Fig. 4

The index i designates the particle history. The temperatures in the various zones are then obtained from the following difference version of Eq. (12):

$$T_{j-2}^{n+1} = T_{j-2}^n + \frac{c \Delta t}{\rho c} \left[\left(T_{j-2}^{n+\frac{1}{2}} \right)^2 - \left(T_{j-2}^n \right)^2 - \sum_i E_{ij-2}^{n+\frac{1}{2}} / \Delta x \right], \quad (57)$$

where $T_{j-2}^{n+\frac{1}{2}}$ is defined as in Eq. (56).

Equation (57) may be solved by a suitable iteration method, e. g., the Newton-Raphson method. The entire Monte Carlo method of solving the transport and energy equations is briefly summarized by the flow diagram, Fig. 4.

V. NUMERICAL RESULTS

There are four questions connected with the Monte Carlo calculation which merit special consideration.

1. The first is the question of convergence. Because of the rather unique combination of a Monte Carlo with a finite difference calculation there is no assurance that the numerical solutions will converge to the actual solutions of the differential equations.

2. The second is the question of statistical accuracy. An important part of any Monte Carlo calculation is estimating the variance of the quantities which are being averaged over the population of histories. Due to the intricate way in which the Monte Carlo histories calculated during a given time cycle depend on those calculated during previous time cycles, a meaningful variance estimate valid beyond the first time cycle seems out of the question.

3. Thirdly there is the question of errors other than statistical errors, i. e., truncation errors. These errors will in all likelihood be influenced by statistical errors.

4. Finally the question of stability needs to be considered. The situation is complicated in this respect by the addition of statistical errors to round-off errors. In addition to the usual possibility of the growth of round-off errors, the possibility also exists that statistical inaccuracies may contribute to errors which grow with time.

No attempt will be made to answer these questions on a theoretical basis. Instead a purely heuristic approach will be taken. We have at our disposal an alternate numerical method the convergence and stability properties of which are reasonably well understood [see Keller and Wendroff (1956)] and which can be expected to furnish fairly accurate solutions. These solutions in turn can be compared with the Monte Carlo solutions to the same problems. This procedure will furnish answers to the preceding questions in an ad hoc way. We can also apply a consistency check to both types of solution. This will further estimate the accuracy of solutions obtained by both methods. The consistency check is derived as follows:

If Eq. (11) is integrated over μ , the result is

$$\frac{\partial u}{\partial t} + \frac{\partial F}{\partial x} = \kappa \rho (acT^4 - \int_{-1}^1 I d\mu), \quad (58)$$

where $u(x,t)$ is the radiation energy density and $F(x,t)$ is the radiation flux:

$$\begin{aligned} u &= \frac{1}{c} \int_{-1}^1 I d\mu \\ F &= \int_{-1}^1 I\mu d\mu. \end{aligned} \quad (59)$$

If Eq. (58) is combined with Eq. (12), the result is

$$\frac{\partial}{\partial t} (u + \rho c_v T) = - \frac{\partial F}{\partial x}. \quad (60)$$

The integration of Eq. (50), over the volume of the slab and over time yields

$$\int_0^L (u + \rho c_v T) dx = \int_0^t [F(0,t) - F(L,t)] dt \quad (61)$$

which equates the energy content of the slab with the net energy transferred through the faces. The quantity

$$\epsilon = \frac{\epsilon_P^{n+\frac{1}{2}} - \sum_{j=1}^J \left(u_{j-\frac{1}{2}}^{n+\frac{1}{2}} + \rho c_v T_{j-\frac{1}{2}}^{n+\frac{1}{2}} \right)}{\epsilon_P^{n+\frac{1}{2}}} \quad (62)$$

called the "energy check" represents the fractional deviation of the calculated energy in the slab from the calculated net energy pumped in, and provides a useful figure of merit for the accuracy of a calculation. This applies both to the Monte Carlo and to the S_n method.

The "characteristic" S_n method has been coded for an IBM 7090 computer and the Monte Carlo method for the LARC computer at Livermore. In the latter code the LARC's buffering facilities are used to read in and out of fast memory from drum storage the particle data. Blocks of 2500 words may be read into and out of internal storage while calculation is in progress. Thus even though the particle data are stored in drum storage, the access time is that of fast memory.

Results are exhibited in Figs. 5 through 15. In these calculations the units of length are cm, the units of time are such that $c = 1$, the units of energy and temperature are such that $a = 1$, $\rho c_v = 0.5917$, and $T_0 = 1$. Figures 5 and 6 show a comparison between an S_n calculation with eight directions (S_8) and a Monte Carlo calculation. Exhibited are the temperature and radiation energy density u as a function of position at time $t = 40$. In this

Fig. 5. Comparison of S_8 and Monte Carlo temperature distributions for constant mean free path.

Fig. 6. Comparison of radiation energy density for S_8 and Monte Carlo at constant mean free path.

problem $\rho\kappa = 1$, $\sigma_s = 0$, $\Delta x = \Delta t = 0.2$, $L = 20$. This problem in the following discussion will be referred to as problem A.

Both figures show that the S_8 calculation allows energy to penetrate farther into the slab than does the Monte Carlo calculation for the same Δx and Δt . This fact is consistent with the negative value of ϵ (too much energy) for S_8 and the positive ϵ (too little energy) for the Monte Carlo calculations. One would conclude that the Monte Carlo results are more accurate on the basis of the smaller magnitude of the energy check associated with it. This conclusion is further substantiated when the Δt and Δx are refined to 0.1 and 0.1 for the S_8 calculation. In this case the ϵ is reduced to -4% at $t = 40$, and the two curves are brought closer together (see Fig. 7). Also shown in Fig. 5 is the temperature distribution for $\Delta x = \Delta t = 1$. The larger zoning and time cycle lead to an ϵ of 25%. Figure 8 shows a comparison of two S_8 calculations, one for $\Delta t = \Delta x = 0.2$ the other for $\Delta t = \Delta x = 1$. The coarser-zoned case results in $\epsilon = 86\%$. The loss of accuracy is evident in the plotted points.

The superior accuracy of the Monte Carlo method over the S_n method is due to the fact that the Monte Carlo method conserves energy regardless of zone size, whereas in the "characteristics" S_n method energy is not very well conserved except for small zones and short time cycles.

It has already been mentioned that variance estimation appears to be out of the question. However, some qualitative insight into the statistical accuracy of the Monte Carlo calculation can be gained by comparing solutions to the same problem obtained with different sets of random numbers and different numbers of histories. Figures 9 and 10 show the energy checks for problem A using 1000 and 5000 source particles per time cycle respectively for the first 50 cycles. It will be noticed that not only is the spread

Fig. 7. Temperature distributions for S_8 and Monte Carlo.

Fig. 8. Comparison of two S_8 runs with different zoning.

Fig. 9. Energy check as a function of time cycle for 1000 source particles.

Fig. 10. Energy check as a function of time cycle for 5000 source particles.

in ϵ for the case of 5000 source particles smaller, but ϵ is generally smaller in magnitude as well. This superiority however was only temporary. The energy checks for the 5000-source-particle case after 170 cycles changed sign and increased in magnitude to an average value of about 4% by cycle 200. The energy checks in the 1000-source-particle case (not shown) past cycle 200 were also of the same order of magnitude but exhibited somewhat greater spread.

A comparison of the temperature distributions for two Monte Carlo runs on problem A using 5000 source particles per cycle is shown in Fig. 11. The time corresponds to 200 cycles. The agreement is good and it appears that if smooth curves were drawn through the two sets of data they would be almost indistinguishable. The energy penetration E_p defined by

$$E_p = \int_0^t [F(0,t) - F(L,t)] dt \quad (63)$$

has values of 4.6398 and 4.6159 (in arbitrary units) for the two cases — which is agreement within 1/2%. Energy penetrations as a function of time are shown in Fig. 12 for four different cases involving different sets of random numbers: the two runs of problem A with 5000 source particles per cycle and the two runs for problem B which differs from problem A in setting $\Delta x = \Delta t = 1$. At time 40 the two curves for problem B agree to within 3/4%. However, $t = 40$ corresponds to only 40 cycles for problem B. After this time the gap between the two B curves widens substantially. This gap also shows fluctuations in size. An interesting feature of the B curves is that they never cross. Once the trend is established it does not seem to reverse itself. The same is true of the A curves although this effect cannot be distinguished on the figure.

Fig. 11. Comparison of two Monte Carlo runs with different sets of random numbers.

The effect of introducing scattering is shown in Fig. 13. In this problem $\kappa\rho = 1/2$, $\sigma_s = 1/2$, $\Delta x = 0.2$. The total mean free path is thus the same as in problem A. Differences from the results of problem A are difficult to distinguish and appear to lie within the bounds of statistical error. It does appear, however, that at least below the knee of the curve the scattering results are lower at a given value of x . In Fig. 14, which shows a comparison of the same solutions obtained by the S_N method, the effect is clearly noticeable.

In Fig. 15 the temperature distribution has been allowed to come to equilibrium for the following problem: $\Delta x = 0.2$, $L = 5$, $\sigma_s = 0.5$, $\kappa\rho = 1/(T + 0.1)$. This problem might be thought of as applying to a stellar atmosphere with both scattering and absorbing properties. Once the equilibrium temperature distribution has been determined in this grey case, the source function $B_\nu(T)$ which appears in Eq. (11) can be calculated. The steady-state transport equation with a known source $B_\nu(T)$ can be solved by known techniques (see ref. 3) for the frequency-dependent radiation intensity I_ν . The importance of the Monte Carlo method in the present application is that it can, at least in principle, be readily generalized to take into account the effect of a frequency-dependent absorption coefficient $\kappa_\nu\rho$ on the temperature distribution and the resulting intensity I_ν . It should also be of use when detailed processes, e. g., the polarization of light, become important.

VI. SUMMARY AND CONCLUSIONS

A method has been described for calculating both time-dependent and steady-state nonlinear radiative transfer by means of a Monte Carlo method. The method is presumably applicable to other nonlinear transport problems provided that there exist suitable variables whose changes can be calculated from finite difference equations coupled in a suitable way to the Monte Carlo

Fig. 13. Comparison of Monte Carlo runs for constant mean free path with and without scattering.

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Fig. 14. Comparison of S_n runs for constant mean free path with and without scattering.

calculations. In testing the method it has been found to yield good agreement with purely finite difference methods. Although no method has been devised to estimate variances for the method, it has been possible to achieve a reasonable degree of reproducibility using different sets of random numbers. Furthermore, it has been demonstrated that problems of reasonable length can be run without an appreciable buildup of errors, statistical or otherwise.

Fig. 15. Monte Carlo and S_n runs for mean free path depending on temperature.

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