JOURNAL OF COMPUTATIONAL PHYSICS 54, 508–523 (1984)

# A Random Walk Procedure for Improving the Computational Efficiency of the Implicit Monte Carlo Method for Nonlinear Radiation Transport*

J. A. FLECK, JR., AND E. H. CANFIELD

*University of California,*
*Lawrence Livermore National Laboratory, Livermore, California 94550*

Received July 27, 1983; revised October 19, 1983

An unconditionally stable Monte Carlo method for solving the frequency dependent equations of nonlinear radiation transport has been described previously. One of the central features of this method is the replacement of a portion of the absorption and reemission of radiation by a scattering process. While the inclusion of this scattering process assures the accuracy and stability of solutions regardless of local opacity values, it becomes time consuming when the local opacity is large. A procedure is derived for replacing a large number of local scattering events by a single advance of the coordinates and time of a particle. This procedure, developed by appealing to the theory of random flights, is integrated into the implicit Monte Carlo scheme and is invoked only when certain conditions are met. Numerical tests indicate that the random walk procedure can substantially improve the computational efficiency of the implicit Monte Carlo method without affecting its accuracy. This random walk procedure with suitable modifications should be applicable to the Monte Carlo solution of other transport problems involving large amounts of scattering.

## 1. INTRODUCTION

The implicit Monte Carlo method [1] provides accurate and unconditionally stable numerical solutions to a wide class of time-dependent nonlinear radiation transport problems, which can arise in astrophysics or in the description of high temperature laser produced plasmas. It furthermore applies equally well to optically thin or optically thick media, or any combination of the two, without compromising accuracy. Despite the unconditional stability of the method it can prove time consuming when applied to optically thick media. In this paper we describe a method that can improve its efficiency substantially under such circumstances. While the specifics of the method have been tailored to radiation transport applications, it should be applicable with suitable modifications to a variety of other transport problems that involve a significant amount of scattering.

* Work performed under the auspices of the U. S. Department of Energy by the Lawrence Livermore National Laboratory Contract W-7405-ENG-48.



0021-9991/84 $3.00

In the explicit Monte Carlo solution of nonlinear radiation transport problem [2] radiation energy bundles are generated from the local temperature dependent emission sources and followed to extinction either by absorption or leakage from the system. Energy changes in the radiation field are subsequently balanced against those of the matter. This method works well in optically thin media but due to its conditional stability requires unacceptably short time steps and fine spatial zoning for problems involving optically thick media. The limitations of the explicit scheme are well known.

In the implicit Monte Carlo scheme, on the other hand, a fraction of the absorption processes are replaced by scattering events, which represent the absorption and reemission of radiation; the longer the duration of the integration time step $\Delta t$ and the larger the local Planck mean absorption coefficient the greater is the fraction. In addition to unconditional stability this scattering process provides a number of other calculational advantages, which include near balance between emission and absorption in optically thick media, economy of source particles, good statistics, and accurate spatial definition of sources.

Despite these advantages computational efficiency can suffer when a large number of scattering events is required to transport radiation particles across regions of high opacity. In such situations one would like to be able to simulate the resulting complex flight paths by a simple random walk algorithm, based on the statistical properties of the scattering process [3].

In this paper we shall derive such a random walk procedure capable of representing a large number of scattering steps by a single advance of the coordinates and time of a particle. The procedure is valid for frequency-dependent problems, but frequency plays a role only insofar as frequency-averaged diffusion and absorption coefficients are employed in the random walk procedure. The nature of the random walk procedure is such that it can be invoked anywhere within the geometry of the problem, if the right conditions are met. Thus there is no need to consider separate "diffusion" and "transport" regions. Improvements in efficiency resulting from the random walk procedure can be expected to be highly problem dependent. However, for the illustrative example included in this paper employing random walk can cut problem running times by a factor of 8.

The paper is organized as follows: The basic ingredients of the implicit Monte Carlo method are reviewed in Section 1. The emphasis here is on the working equations and procedures. For derivations the reader is referred to [2]. The statistical properties of the random flights of particles peculiar to the implicit Monte Carlo method are derived in Section 3. These properties are used to derive a diffusion equation that governs the random flights in the limit of a large number of collisions. In Section 4 the statistics of the random flights are used to derive a procedure for shortening the work involved in a practical implicit Monte Carlo calculation. Criteria for applying the procedure are also stated. The treatment of absorption for particles undergoing random flights is derived in Section 5. Numerical results comparing pure implicit Monte Carlo, implicit Monte Carlo combined with random walk, and multigroup diffusion theory are presented in Section 6.

## 2. Review of the Implicit Monte Carlo Method

The basic equations the method is intended to solve are

$$\frac{1}{c}\frac{\partial I_\nu}{\partial t}+\frac{\partial I_\nu}{\partial x}+\sigma_\nu I_\nu=\frac{1}{2}c\sigma_\nu B_\nu, \tag{1a}$$

$$b\frac{\partial T}{\partial t}=\iint \sigma_\nu I_\nu\,dv\,d\mu-c\iint \sigma_\nu B_\nu\,dv\,d\mu+S. \tag{1b}$$

The first equation is the radiative transfer equation under the assumption of local thermodynamic equilibrium, where $I_\nu$ is the specific intensity, $B_\nu$ is the specific intensity of a black body, and $\sigma_\nu$ is the frequency dependent macrosopic absorption cross section. The second equation is the equation of material energy conservation, where $b(T)=\rho c_v$ represents the material specific heat. The first two terms represent radiation absorption and emission rates and $S$ represents an arbitrary source function.

The implicit Monte Carlo procedure for solving Eqs. (1a) and (1b) numerically is based on the following set of equations derived in [1] for advancing the radiation field and material temperature from time $t^n$ to time $t^{n+1}$:

$$\frac{1}{c}\frac{\partial I_\nu}{\partial t}+\frac{\partial I_\nu}{\partial x}+(\sigma_\nu^a+\sigma_\nu^s)\,I_\nu$$
$$=\frac{1}{2}(1-f)(\sigma_\nu b_\nu/\sigma_{\mathrm{P}})\iint \sigma_{\nu'}I_{\nu'}\,dv'\,d\mu'+\frac{1}{2}fc\sigma_\nu b_\nu u_{\mathrm{r}}^n+\frac{1}{2}(1-f)(\sigma_\nu b_\nu/\sigma_{\mathrm{P}})\,S^\gamma, \tag{2a}$$

$$T^{n+1}=T^n+b^{-1}(T)f\left\{\int_{t^n}^{t^{n+1}}dt\iint \sigma_\nu I_\nu\,dv\,d\mu-c\Delta t\sigma_{\mathrm{P}}u_{\mathrm{r}}+S^\gamma\Delta t\right\}, \tag{2b}$$

$$\sigma_\nu^a=f\sigma_\nu, \tag{2c}$$

$$\sigma_\nu^s=(1-f)\,\sigma, \tag{2d}$$

$$f=\frac{1}{1+\alpha\beta c\Delta t\sigma_{\mathrm{P}}}, \tag{2e}$$

$$u_{\mathrm{r}}=aT^4, \tag{2f}$$

$$b_\nu=B_\nu u_{\mathrm{r}}^{-1}, \tag{2g}$$

$$\sigma_{\mathrm{P}}=\int b_\nu\sigma_\nu\,dv, \tag{2h}$$

$$\beta=\left(\frac{\partial u_{\mathrm{r}}}{\partial T}\right)\left(\frac{\partial u_m}{\partial T}\right)^{-1}=4b^{-1}(T)\,aT^3, \tag{2i}$$

$$\Delta t=t^{n+1}-t^n. \tag{2j}$$

Here $u_r$ is the equilibrium radiation energy density, $b_\nu$ is a normalized Planck spectrum, $\sigma_P$ is the Planck mean cross section, $\alpha$ is a centering parameter that has the value 0 for a completely explicit treatment and 1 for a completely implicit treatment, and $S^\gamma$ is the source term appropriately time-centered. The quantity $\beta = 4u_r/bT$ is a measure of the ratio of energy in the equilibrium radiation field to internal energy in the matter. For simplicity Eqs. (1) and (2) have been written for one-dimensional slab geometry, but this does not affect the generality of the discussion. It is assumed that space has been discretized into zones and that the temperature $T$ refers to a typical spatial zone over which temperature and any function of temperature are to be regarded as constant. Unless otherwise indicated the quantities in Eqs. (2a)–(2j) that require time centering refer to time $t = t^n$.

The transfer Eq. (2a) differs from Eq. (1a) by the replacement of a fraction $(1-f)$ of the emission source term by an isotropic energy conserving scattering source and by the division of the true absorption coefficient $\sigma_\nu$ in Eq. (1a) into an absorption part $\sigma_\nu^a = f\sigma_\nu$ and a scattering part $\sigma_\nu^s = (1-f)\sigma_\nu$ that appear in Eq. (2a).

The scattering process in Eq. (2a) has the physical significance of absorption and reemission of radiation, which is made plausible by the observation that radiation emerges from scattering with a normalized emission spectrum $\sigma_\nu b_\nu/\sigma_P$. For an implicit treatment the scattering terms assume increasing importance as the product $\beta\Delta t\sigma_P$ increases. This is as it should be, since for large $\Delta t$ and/or strong absorption it becomes highly probable that any radiation emitted during the current integration cycle will have undergone absorption and reemission at least once. For an explicit treatment, on the other hand, the scattering terms disappear from Eq. (2a) and it is no longer possible to account for the possibility that reemission can follow the absorption of radiation during a cycle time $\Delta t$. Thus, quite apart from stability considerations, an explicit treatment would be expected to give accurate solutions only for values of $\Delta t$ sufficiently small to strongly limit the amount of absorption that can take place in one cycle.

Finally, Eq. (2b) expresses a material energy balance, which equates the gain in the internal energy of matter with the difference between the radiation energy absorbed and the radiation energy emitted during the time $\Delta t$. The factor $f$ has the effect of excluding from the matter energy balance absorbed radiation that has been reradiated. This has a calculational bonus. Near equilibrium the right-hand equation (1b) involves small differences between large sources and sinks, a situation inherently difficult to treat by Monte Carlo. In Eq. (2b), the effect of this noise source is reduced by the factor $f$, often by orders of magnitude.

A Monte Carlo solution [2] of Eqs. (2) requires generation of a population of radiation source particles that correspond to the nonscattering source term on the right side of Eq. (2a). These particles should be distributed uniformly in direction and uniformly in time over the interval $\Delta t$. The total energy weight $W_e$ for source particles generated in a particular zone should be

$$W_e = [fc\sigma_P u_r^n + (1-f)S^\gamma]\,\Delta t\,\Delta x, \tag{3a}$$

and their frequencies should be determined by sampling the distribution $\sigma_\nu b_\nu/\sigma_P$ appropriate to the zone in question. It is essential for the spatial sampling of source particles within a zone to reflect the spatial gradients of $u_r$, if transport into optically thick materials is to be calculated accurately. One such spatial sampling scheme involves selecting $x$ values for particles in the $k$th zone, where $x_{k-1} < x < x_k$, from the unnormaized spatial distribution

$$p_k(x) = \text{const.} \times [u^n_{rk+1} + (u^n_{rk+1} - u^n_{rk-1})]/(x_k - x_{k-1}), \tag{3b}$$

where $u^n_{rk}$ is the constant value of $aT^4$ in the $k$th zone. A more accurate scheme that has been successfully implemented employs a quadratic spline representation of the zone to zone temperature variation [4]. Since $\sigma_P$ is a rapidly varying function of temperature, it is also essential to employ in Eqs. (2) and (3) values of $\sigma_P$ that are extrapolated to a time consistent with the assumed value of $\alpha$; for example, if $= 1$, $\sigma_P$ should be extrapolated to $t^{n+1}$.

Once generated, source particles are tracked to escape or census. Particles that survive to census are used along with source particles in succeeding cycles. The energy weight of all particles is attenuated by the factor $\exp(-\sigma^a_\nu s)$, where $s$ is the track length between events, and the number of particles is reduced at census by a scheme that favors the retention of only highest weight particles. The energy lost by particles is accumulated during the cycle by zone and at the end of the cycle these totals are added to the material internal energies for the appropriate zones, and the zone temperatures are advanced in accordance with Eq. (2b). Since $b(T)$ is a function of temperature, the upgrading of temperature by Eq. (2b) requires an iterative procedure, if energy is to be strictly conserved.

The fully explicit form of calculation clearly involves less computation per cycle than the implicit scheme, since reemission scattering events are eliminated. The fully explicit scheme, however, can be expected to work stably only if $\Delta t \ll \min(\tau_e)$, where $\tau_e \approx (\beta c \sigma_P)^{-1}$ is the time for equilibration between matter and radiation, and min signifies the minimum value for all zones. This condition can be extremely restrictive if the problem contains even the slightest amount of high opacity material. Thus, many more cycles are required to complete a problem for the explicit scheme and the overall time to complete a problem can be must greater.

The fully implicit form of Eq. (2) with $\alpha = 1$, on the other hand, removes all restrictions on $\Delta t$ for a stable solution and makes it possible to calculate transport in optically thick media with practical length time steps. More important, the implicit method makes it possible to continue a solution from a transparent region into a high-opacity region in a rigorous and self-consistent manner. The scattering terms in Eq. (2a) not only ensure stability but also enhance accuracy by giving accurate spatial definition to the emission sources. The latter feature reduces the sensitivity of calculational results to zone size. A further advantage of the implicit method is that since particles are, in effect, reused through the effective scattering process census, lists can be drastically reduced below those required for explicit calculations.

Despite these advantages of implicit Monte Carlo, the cost of performing the

required scattering events by analog Monte Carlo can become quite onerous when $f \ll 1$ and $\sigma_v$ is large. When a large number of scattering events is likely to take place before census or a boundary crossing, it would be desirable to substitute a single diffusion–random walk event for the complex scattering chain. This does not imply that the problem should be divided into pure transport and diffusion regions. On the contrary, the decision to "shift gears" between transport and random walk should be based on a general set of conditions that can apply anywhere in space and time. This would allow both particles and zones to change their character with time.

## 3. Statistics of a Random Chain of Scattering Events Representing the Absorption and Reemission of Radiation

In this section we derive a set of statistical relationships that characterize the random walk embodied in Eq. (2a). We consider an ensemble of particles that undergo a sequence of isotropic scattering events described by the scattering terms of Eq. (2a). The effects of absorption are ignored here but can be treated separately by an appropriate exponential attenuation along each flight path. This will be the subject of Section 5. The scattering cross section

$$\sigma_v^s = (1 - f)\,\sigma_v \tag{4}$$

is assumed to be independent of position. It is also assumed that the initial direction of a particle is isotropic and that the initial and scattered frequencies are distributed according to the normalized probability density function

$$f(\nu) = \sigma_\nu b_\nu / \sigma_{\mathrm{P}}. \tag{5}$$

The random flight path for a particular particle of the ensemble is illustrated in Fig. 1.

The particle's displacement $\mathbf{r}(N)$ from its initial position following $N$ collisions can be written

$$\mathbf{r}(N) = \sum_{i=1}^{N} \mathbf{R}_i, \tag{6}$$

where each of the individual displacements $\mathbf{R}_i$ is statistically independent but otherwise distributed in the same manner. Note that the vectors $\mathbf{R}_i$ originate at the position of the collision numbered $i - 1$. A statistical description of the random walk requires a calculation of the second moment

$$\langle r^2(N)\rangle = \sum_{i=1}^{N}\sum_{j=1}^{N} \langle \mathbf{R}_i \cdot \mathbf{R}_j\rangle = \sum_{i=1}^{N} \langle R_i^2\rangle = N\langle R^2\rangle, \tag{7}$$

where $R$ is a random variable representing the displacement of a particle between

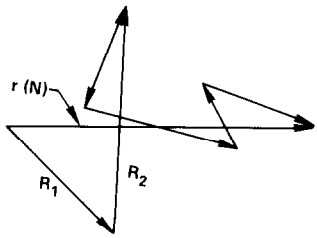


FIG. 1. Random walk involving 6 scattering events. The vector $\mathbf{r}(6)$ represents the total displacement of the particle at the 6th collision.

isotropic scattering events with cross section $\sigma_\nu^s$ and scattered frequency distribution $f(\nu)$.

In order to calculate $\langle R^2 \rangle$ and the expectation values of other functions of $R$ we shall need to know the joint distribution function $f(R, \nu)$, where $f(R, \nu)\, dR\, d\nu$ is the probability that a particle will scatter into frequency $\nu$ and travel a distance $R$ before its next collision. Let $f(R \mid \nu)$ represent the conditional probability that a particle with frequency $\nu$ will travel a distance $R$ before undergoing a collision. From elementary collision theory we must have

$$f(R \mid \nu)\, dR = \exp(-\sigma_\nu^s R)\, dR. \tag{8}$$

From the definition of a joint probability distribution

$$f(R, \nu) = f(r \mid \nu) f(\nu) = \exp(-\sigma_\nu^s R) \left( \frac{\sigma_\nu^s \sigma_\nu b_\nu)}{\sigma_P} \right). \tag{9}$$

The expected value $\langle g(R) \rangle$ for some general function of $R$ is

$$\langle g(R) \rangle = \int_0^\infty d\nu \int_0^\infty g(R) f(R, \nu)\, dR = \int_0^\infty d\nu \frac{\sigma_\nu^s \sigma_\nu b_\nu}{\sigma_P} \int_0^\infty g(R) \exp(-\sigma_\nu^s R)\, dR. \tag{10}$$

For example,

$$\langle R \rangle = \int_0^\infty d\nu \frac{b_\nu}{\sigma_P} \int_0^\infty \frac{R}{(1-f)} (\sigma_\nu^s)^2 \exp(-\sigma_\nu^s R)\, dR = \frac{1}{(1-f)\, \sigma_p}, \tag{11}$$

where use has been made of Eq. (4). Thus, the mean distance travelled between collisions is $\sigma_P^{-1}/(1-f)$ or $\lambda_P/(1-f)$, where $\lambda_P$ is the Planck averaged mean free path. Correspondingly, the mean time $\tau_c$ between collisions is $\langle R \rangle / c$ or

$$\tau_c = \frac{1}{(1-f)\, \sigma_P c} = \frac{\lambda_P}{(1-f)\, c}. \tag{12}$$

Let us now compute the second moment $\langle R^2 \rangle$. From Eq. (11) we have

$$\langle R^2 \rangle = \int_0^\infty dv \frac{b_v}{\sigma_P} \int_0^\infty R^2 \sigma_v^s \sigma_v \exp(-\sigma_v^s R)\, dR$$

$$= \frac{2}{(1-f)^2 \sigma_P} \int_0^\infty dv \frac{b_v}{\sigma_v} = \frac{2}{(1-f)^2 \sigma_P \sigma_R}, \tag{13}$$

where the mean free path $\sigma_R^{-1}$ is computed as the average of $\sigma_v^{-1}$ over a normalized Planck distribution. This computation, as the subscript R indicates, is suggestive of the Rosseland mean free path, computed as $\sigma_v^{-1}$, averaged over the frequency distribution $\partial B_v(T)/\partial T$. The cross section $\sigma_R$ is sometimes referred to as the Planck reciprocal mean cross section, or simply, the reciprocal mean cross section.

Returning to Eq. (7) we have

$$\langle r^2(N) \rangle = N \langle R^2 \rangle = \frac{2N}{(1-f)^2 \sigma_P \sigma_R}. \tag{14}$$

This result can now be used to calculate a diffusion constant $D$. In the limit of a large number of collisions $N$, the probability density function for the distribution of a particle's coordinates becomes [5]

$$\psi(\mathbf{r}, N) = \frac{1}{(2\pi N \langle R^2 \rangle / 3)^{3/2}} \exp(-3r^2 / 2N \langle R^2 \rangle), \tag{15}$$

where $\mathbf{r} = (x, y, z)$. The above expression can be identified as the solution of the diffusion equation

$$\frac{\partial \psi}{\partial t} = D \nabla^2 \psi, \tag{16}$$

for an unbounded medium, subject to the initial condition

$$\psi(\mathbf{r}, t) = \delta(\mathbf{r}). \tag{17}$$

The latter solution is

$$\psi(\mathbf{r}, t) = \frac{1}{(4\pi D t)^{3/2}} \exp(-r^2 / 4\mathrm{D}t). \tag{18}$$

Comparing Eqs. (15) and (18), one obtains

$$N \langle R^2 \rangle = 6Dt. \tag{19}$$

If we identify

$$t = N\tau_c, \tag{20}$$

$D$ can be expressed as,

$$D = \langle R^2 \rangle / 6\tau_c = c/3(1-f)\,\sigma_R, \tag{21}$$

where use has been made of Eqs. (12) and (14). When large numbers of collisions are involved, one can obtain the probability density function for the scattered particles by solving Eq. (16) directly without further reference to the details of the collisions.

## 4. Application of Random Flight Statistics to Implicit Monte Carlo

Having derived the necessary statistical properties of the random flights, we now develop a random walk procedure for shortening the work in implicit Monte Carlo transport. We first determine criteria that must be satisfied before the random walk procedure can be invoked. Since the particles considered in Section 3 were distributed uniformly in direction and in frequency according to the emission function in Eq. (5), we can include only source particles, or nonsource particles that have undergone at least one collision in the zone of interest. Particles that enter the zone of interest and pass right through without a collision need not be considered. These three possibilities are illustrated in Fig. 2.

We shall further restrict our attention to random flight paths that are confined to some limited spatial region contained entirely within one zone. For simplicity we assume this region to be the largest sphere, with radius $R_0$, centered at the starting position of the particle that can fit inside the zone (see Fig. 3). In order to aply diffusion theory to random flights it is necessary for a sufficient number of scattering

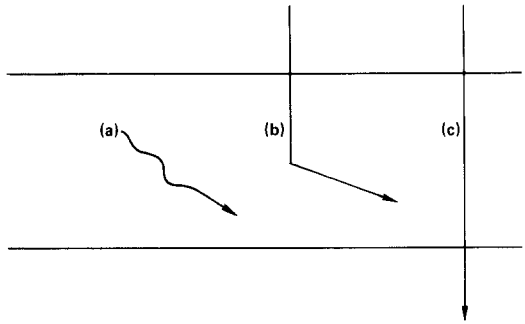


Fig. 2. Three classes of particles that are considered in applying statistics of random flights to implicit Monte Carlo radiation transport: (a) particle generated within zone from emission source, (b) scattered particle representing absorption and reemission, (c) particle generated in another zone that passes through without absorption and reemission scattering. Only particles in classes (a) and (b) need be considered for the application of random walk theory.

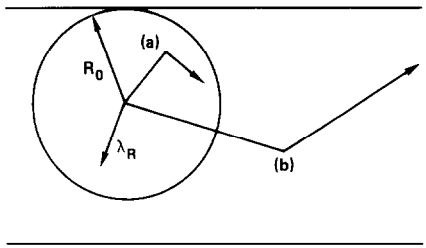


FIG. 3. Random walk theory is applied to random flight paths that are confined to a limited spatial region. For the example depicted here the region is a sphere of radius $R_0$ tangent to one zone boundary. Two scattering cases are shown: (a) inside sphere (b) outside sphere. If $R_0 > \lambda_R$ and case (a) applies, random walk theory is invoked.

events to take place. While the following heuristic criteria do not rigorously guarantee the applicability of diffusion theory, they have in practice led to very good results:

$$R_0 > \lambda_R, \tag{22}$$

$$d_{COL} = |\ln u|/\sigma_t^s < R_0, \tag{23}$$

where $d_{COL}$ is the distance to the next collision and $u$ is a random number distributed uniformly in the interval 0 to 1. The first criterion guarantees that the particle will move at least one "Rosseland" mean free path within the sphere. Since $\lambda_P$ tends to be much less than $\lambda_R$, and $\lambda_p$ is the mean distance between collisions, condition (22) could imply many collisions. The second criterion guarantees that the particle with its current frequency will collide inside the sphere at least once. If neither criterion is fulfilled, the particle is tracked by the conventional rules of Monte Carlo transport. The possible outcomes are shown in Fig. 4.

As pointed out in Section 3, the probability density for the position of a particle is governed by Eqs. (16) and (17) in the limit of a large number of collisions. The solution (18), however, is valid only for an unrestricted set of random walks in an

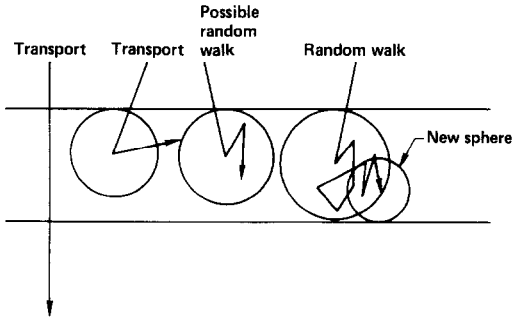


FIG. 4. Procedure for combining random walk with implicit Monte Carlo allows for either analog transport or random walk, depending on whether certain criteria are met.

infinite medium. We are interested in the probability density governing a more restricted class of random walks that terminate before the particle can leave the confines of the sphere in question. The latter probability distribution can be determined, if we impose a perfectly absorbing barrier at the surface of the sphere. We must, therefore, solve Eq. (16) subject to the boundary condition

$$\psi(r = R_0, t) = 0, \tag{26}$$

which implies that particles arriving at the surface of the sphere are incapable of further displacements. Application of Eq. (16) with the boundary condition (26) requires one approximating assumption, namely, that the diffusion constant $D$, derived as an average over an infinite range of distances between collisions applies when the collisions are confined to the interior of the sphere. Again, this will be a good approximation for those chains involving a large number of collisions, which condition (22) and (23) were designed to select.

The solution of Eq. (16) subject to initial and boundary conditions (18) and (26) can be expressed in the form

$$\psi(r, t) = \frac{1}{2R_0^2} \sum_{n=1}^{\infty} \left(\frac{n}{r}\right) \exp\left\{-\left(\frac{\pi n}{R_0}\right)^2 Dt\right\} \sin\left(\frac{n\pi r}{R_0}\right). \tag{27}$$

The probability $P_R(t)$ of a particle remaining entirely within the sphere for a time $t$ is

$$P_R(t) = 2\pi \int_0^{R_0} \psi(r, t)\, r\, dr, \tag{28}$$

whereas the probability of the particle arriving at the surface of the sphere and terminating its random walk is

$$P_T(t) = 1 - P_R(t) = 1 - 2\pi \int_0^{R_0} \psi(r, t)\, r\, dr. \tag{29}$$

Equations (27)–(29) form the basis of the Monte Carlo random walk procedure, which is invoked when conditions (23) are satisfied. The first step is to determine whether the random flight chain has terminated with the particle reaching the surface of the sphere before census time, or whether the flight chain will be continued into the next integration cycle. (In the latter case the particle is moved to a new position in the sphere and retired to census.) One of these possibilities is decided by the outcome of

$$0 < u \leqslant P_T(t_{CEN}) \qquad \text{particle reaches surface before census,} \tag{30a}$$

$$P_T(t_{CEN}) < u \leqslant 1 \qquad \text{particle still in sphere at census.} \tag{30b}$$

The comparisons (30) are best accomplished using a one-dimensional table of values of $P_T(t)$.

If the more likely of the two outcomes (30a) is satisfied, the actual time $t_T$ at which the random flight chain is terminated is found by solving the equation

$$P_T(t_T) = u \tag{31}$$

by table lookup, where $u$ is the same random number that satisfies Eq. (30a). The clock of the particle is then advanced to $t + t_T$, and the new position of the particle is selected from a distribution that is uniform on the surface of the sphere, $r = R_0$.

The random walk is completed when the particle is assigned a new frequency and direction. We recall that the statistical analysis of Section 3 leading to a diffusion equation was based on observations of particles immediately following collision events. This would lead us to conclude that in the limit that diffusion theory accurately describes the random flights, the frequencies and directions of the terminated particles should be distributed in the same manner as scattered particles, that is, their frequencies should be distributed according to Eq. (5), and their directions should be distributed uniformly in solid angle. However, it is necessary to bear in mind that any particle that reaches the sphere by a random scattering chain must have undergone its last collision inside the sphere. Thus it is more accurate to assign the new particle direction from a cosine distribution about the local normal to the sphere. The accuracy of this assumption has been empirically verified by computation.

If condition (30b) is satisfied, the particle is given a new direction and position and advanced to census. The new direction is selected from a uniform distribution and the new position is uniformly distributed on the surface of the sphere $r = R_1$, where $R_1$ is computed by solving the equation

$$2\pi \int_0^{R_1} \psi(r, t_{CEN})\, r\, dr = u' P_R(t_{CEN}), \tag{32}$$

where $u'$ is a new random number. Equation (32) is best solved by means of a two-dimensional table lookup.

## 5. Treatment of Absorption

Scattering can be treated independently of absorption, provided that at the end of a multiple collision path the radiation particle weight is multiplied by the factor

$$W_N = \prod_{i=1}^{N} \exp(-f\sigma_i R_i), \tag{33}$$

where $R_i$ is the length of the $i$th segment between scattering events, and $\sigma_i = \sigma_v$ for the frequency appropriate to the same segment. It will be assumed that all of the collisions referred to in Eq. (33) take place within the same zone.

We now wish to calculate the ensemble average

$$\langle W_N \rangle = \left\langle \sum_{i=1}^{N} \exp(-f_i R_i) \right\rangle = \langle \exp(-f\sigma_\nu R) \rangle^N, \tag{34}$$

where use is made of the statistical independence of each path segment. From Eq. (11) we have

$$\begin{aligned} \langle \exp(-f\sigma_n R) \rangle^N &= \left\{ \int_0^\infty \frac{\sigma_\nu b_\nu}{\sigma_p} d\nu \int_0^\infty \exp(-\sigma_\nu R)(1-f)\,\sigma_\nu\, dR \right\}^N \\ &= (1-f)^N \\ &= \exp[N \ln(1-f)] \end{aligned} \tag{35}$$

If use is made of Eqs. (21) and (13), one can write Eq. (35) as

$$\langle \exp(-f\sigma_\nu R) \rangle^N = \exp\{(1-f)\ln(1-f)\,\sigma_{\mathrm{P}} ct\}. \tag{36}$$

This means that the weight factor $\langle W_N \rangle$ can be expressed as

$$\langle W_N \rangle = \exp(-c\sigma^a_{\mathrm{eff}} t), \tag{37}$$

where $t$ is the time elapsed in the random walk and

$$\sigma^a_{\mathrm{eff}} = (1-f)\ln(1-f)^{-1}\,\sigma_{\mathrm{P}}. \tag{38}$$

For $f \ll 1$, Eq. (38) can be approximated by

$$\sigma^a_{\mathrm{eff}} \cong f\sigma_{\mathrm{P}}. \tag{39}$$

## 6. Numerical Examples

It is assumed that radiation from a 1.0 keV blackbody impinges on a slab of lead from one side. The incident radiation is distributed in frequency according to a Planck spectrum and in direction with a cosine distribution about the normal to the slab. Figures 5 and 6 show the net energy penetration into the slab as a function of time under the assumption that the blackbody is turned on instantaneously at $t = 0$.

Displayed in Fig. 5 are results for diffusion theory, pure implicit Monte Carlo, and inplicit Monte Carlo combined with the random walk procedure previously derived. The diffusion calculation was carried out with 50 frequency groups, while the cross sections employed with both Monte Carlo calculations were defined by 128 groups. The discrepancy in the number of groups is not considered to be important. Each method was applied with a zone density of 32 zones per mm of penetration depth, which is sufficient to ensure accurate results. Monte Carlo results were obtained with a quadratic spline representation of the temperature [4], which in turn was used to

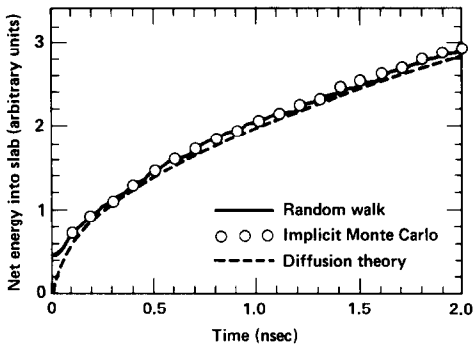


FIG. 5. Radiation energy penetration into a slab from blackbody source on one side, calculated as a function of time with multigroup diffusion theory, implicit Monte Carlo, and implicit Monte Carlo with random walk. Fine zoning is employed with 32 zones/mm.

compute the spatial dependence of the source terms in Eqs. (2a) and (2b). The number of particles at the end of the problem was of the order of 1000.

The three methods give results that are in very good agreement. For the implicit Monte Carlo–random walk combination, however, the small zone size prohibits invoking the random walk procedure often enough for a substantial reduction in running time. This can be seen from Table I, which gives comparative running times as a function of zone density for the two Monte Carlo methods. For Fig. 5 the reduction in running time is about 20 per cent.

Figure 6 shows results for implicit Monte Carlo with and without the random walk procedure for 4 zones/mm. The results in Fig. 6 display a somewhat higher degree of statistical variation than their counterparts in Fig. 5. This behavior is representative of a general tendency observed in the series of calculations for increased statistical noise in the calculated energy deposition to accompany an increase in zone size. The agreement between the two Monte Carlo methods, nonetheless, is quite good

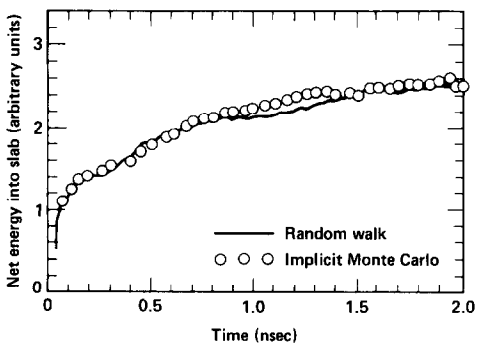


FIG. 6. Radiation penetration into a slab as a function of time for coarse zoning (4 zones/mm). Plotted are results for pure implicit Monte Carlo and implicit Monte Carlo–random walk combination. The latter results in a reduction of running time by factor of 8.6.

TABLE I

Comparison of Running Times as a Function of Zone Size
for Problem of Radiation Penetrating a Lead Slab

| Zone Density (zones/mm) | IMC (min) | IRW (min) | IMC/IRW |
|---|---|---|---|
| 32 | 7.74 | 6.43 | 1.2 |
| 16 | 6.69 | 3.07 | 2.2 |
| 8 | 5.43 | 1.25 | 4.3 |
| 4 | 6.34 | 0.62 | 8.6 |

*Note.* Given are running times for pure implicit Monte Carlo (IMC) and implicit Monte Carlo combined with random walk (IRW).

considering the statistical nature of the results. The inclusion of the random walk procedure for the case of Fig. 6 reduces running time by a factor of 8.6.

One would expect the coarseness in zone size to reduce the accuracy of the results in Fig. 6 relative to those in Fig. 5. Actually, the differences between Figs. 6 and 5 are not appreciable and may be attributed at least in part to statistics. The need for relatively coarse zoning to increase the effectiveness of the random walk procedure makes it all the more important to accurately characterize the spatial dependence of the source terms in Eqs. (2a) and (2b).

## 7. Summary and Conclusion

We have derived a random walk procedure capable of representing a large number of scattering events by a single advance of the coordinates and time of a Monte Carlo particle. Such scattering events represent the absorption and reemission of radiation. This random walk procedure can in turn be integrated into the general implicit Monte Carlo method of radiation transport without compromising its accuracy in situations where strict transport theory is required.

In optically thick regions of a problem where diffusion theory is valid the random walk procedure can significantly increase the computational efficiency of the implicit Monte Carlo method without loss of accuracy. Significant increases in computational efficiency due to the random walk procedure, however, require zoning that is sufficiently coarse for the random walk option to be invoked frequently. In order to achieve accurate results and computational efficiency at the same time it is thus necessary to represent the spatial dependence of radiation source terms as accurately as possible.

## REFERENCES

1. J. A. FLECK, JR. AND J. D. CUMMINGS, *J. Comput. Phys.* **8** (1971), 313.
2. J. A. FLECK, JR., *in* "Computational Methods in the Physical Sciences" (B. Alder and S. Fernbach, Eds.), Vol. 1, p. 43, McGraw–Hill, New York, 1963.
3. A method based on the renormalization group has been proposed, although numerical results have not yet been obtained. See G. F. CHAPLINE, *Phys. Rev. A* **21** (1980), 1263.
4. E. H. CANFIELD, unpublished.
5. S. CHANDRASEKHAR, *Rev. Modern Phys.* **15** (1943), 1.