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MONTE CARLO METHOD FOR RADIATIVE TRANSFER†

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Abstract—A Monte Carlo method for the numerical solution of nonlinear, frequency-dependent, radiative transfer problems is described. The accuracy of the method is investigated with respect to the number of particles required, propagation of statistical error, truncation error and convergence to a known solution. The solution of a simple frequency-dependent radiative heating problem is illustrated. Gray-body calculations using both the Planck mean absorption coefficient and the Rosseland mean free path are compared with the frequency-dependent calculation.

NOMENCLATURE

a, radiation constant $8\pi^5k^4/15c^3h^3$;
$B^\nu(T)$, Planck function;
c, velocity of light;
c_v, specific heat at constant volume;
e, base of natural logarithms;
$E_m(T)$, material energy density;
E_p, energy of particle p;
$E^\nu(r, t)$, radiation energy density;
$F^\nu(r, t)$, r component of radiation flux vector;
E, F, corresponding frequency integrated quantities;
h, Planck's constant;
$I^\nu(r, \mu, t)$, the monochromatic specific intensity of radiation;
$I(r, \mu, t)$, the frequency integrated intensity;
j, zone number in the space mesh;
J, maximum number of zones;
k, Boltzmann constant;
$K(\mu, \mu')$, scattering kernel;
N, number of particles;
$P^\nu(r, t)$, rr component of radiation pressure tensor;
r, position coordinate;
$S_p(j)$, distance travelled in zone j by particle p;
S_{bdy}, distance to zone boundary along the particle path;
S_{cen}, distance to census;
S_{enc}, distance to encounter;
t, time;
T, temperature;
T^*, first approximation to $T^{n+\frac{1}{2}}$;
u, random variable in the interval (0, 1);
x, position coordinate.

Greek symbols

α, geometry index;
$\delta_p(j)$, zone indicator for particle p;
$\Delta E_{abs}(j)$, energy absorbed in zone j on the time step Δt;
$\Delta r, \Delta x$, small increments of position;
Δt, time increment;
ΔV_j, volume of zone j;
ϵ, index of energy conservation;
$\bar{\epsilon}$, the time average of ϵ;
λ, mean free path;
λ_R, Rosseland mean free path;
μ, direction cosine relative to the r axis;
ν, frequency of radiation;
ρ, mass density;
σ_a, absorption cross-section in units of (length)$^{-1}$;

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σ_s, scattering cross-section;
$\bar{\sigma}_p$, Planck mean absorption cross-section.

Subscripts

0, indicates a given reference value which is constant;
j, refers to the mesh position $r_j = j\,\Delta r$;
$j + \frac{1}{2}$, refers to the center of zone j;
p, refers to particle p.

Superscripts

v, frequency index (absence of superscript v indicates the corresponding frequency integrated quantity);
n, refers to time $t^n = n\,\Delta t$.

1. INTRODUCTION

THE LAST several years have brought an increasing need for the development of more powerful methods for the numerical computation of nonlinear, frequency-dependent radiation transport. Two fundamentally different procedures are available: the Monte Carlo method, based on a discrete representation of the radiation field; and finite difference methods, based on a continuous representation. The Monte Carlo method is a direct simulation of the physical system by means of statistical sampling. In finite difference methods, the set of nonlinear integro-differential equations which define the system are approximated by finite difference equations on a net of points covering the region in which the solution is required.

In computer methods, the nonlinear character of the problem presents little difficulty. The critical aspects of the problem are the presence of complicated geometrical configurations and the large variation and considerable complexity of the cross-sections. Although finite difference schemes have been developed to handle large variations in cross-section [1, 2], the Monte Carlo method is particularly well-adapted to deal with both aspects of the problem. The Monte Carlo method is limited, by its statistical nature, to calculations where high accuracy is not required. Thus, the source of the great power of the method is also the source of its essential limitation.

Until recently, Monte Carlo techniques were applied only to linear transport calculations. A bibliography of early Monte Carlo work is given by Kraft and Wensrich [3]. For an excellent review of more recent work, including some nonlinear applications, refer to Howell [4]. A basic Monte Carlo method for nonlinear radiative transfer is outlined in this paper. A more complete account, including detailed flow charts, is given by Campbell and Nelson [5]. For those readers unfamiliar with basic Monte Carlo concepts, the work of Kahn [6] is recommended.

2. FORMULATION OF THE PROBLEM

To define the scope of this paper, the following formulation of the nonlinear radiative heating problem is given. This formulation, although not complete, is both general and simple enough to provide a convenient vehicle for the study of basic transport methods.

Under the restrictions of local thermodynamic equilibrium and conservative scattering, the transport equation for one-dimensional symmetry becomes

$$\frac{1}{c}\frac{\partial I^v}{\partial t} + \mu\frac{\partial I^v}{\partial r} + \frac{\alpha}{2}\frac{(1-\mu^2)}{r}\frac{\partial I^v}{\partial \mu} + (\sigma_a^v + \sigma_s)I^v = \sigma_a^v B^v(T) + \sigma_s \int_{-1}^{1} K(\mu, \mu')I^v(\mu')\,d\mu' \quad (1)$$

where $\alpha = 0$ for plane geometry and $\alpha = 2$ for spherical geometry.

To evaluate the temperature-dependent cross-sections and the Planck function, $B^v(T)$, one must keep an account of the energy exchange between the radiation field and the material. When equation (1) is multiplied by 2π and integrated over all μ and v, the conservative scattering terms drop out with the result

$$\frac{\partial E}{\partial t} + \frac{1}{r^\alpha}\frac{\partial}{\partial r}(r^\alpha F) = \int_0^\infty c\sigma_a^\nu \left(\frac{4\pi}{c} B^\nu(T) - E^\nu\right) d\nu = -\frac{\partial E_m(T)}{\partial t} \quad (2)$$

where $E_m(T)$ is the material energy density.

The material energy density must be expressed in terms of the temperature T by an equation of state. A simple example is the ideal gas equation of state,

$$E_m(T) = \rho c_v T \quad (3)$$

where ρ is the mass density and c_v the specific heat.

The transport equation (1) and the appropriate boundary conditions, together with the energy balance equations (2) and the equation of state (3), constitute the complete set of basic relations which define the problem to be considered in this study.

3. BASIC STRUCTURE OF THE METHOD

We superpose upon the region of interest $[0 \leqslant r \leqslant r_{\max}, 0 \leqslant t]$ a rectangular mesh,

$$[r_j = j\,\Delta r, j = 0, 1, 2, \ldots, J; \quad t^n = n\,\Delta t, n = 0, 1, 2, \ldots]. \quad (4)$$

The procedure is to construct within the mesh a Monte Carlo algorithm of the solution to the transport equation (1).

"Particles", groups of photons with common properties, are emitted throughout each space–time zone $[r_j, \Delta r; t^n, \Delta t]$, as determined by the emission function $\sigma_a^\nu B^\nu(T)$ evaluated at the zone center. Particles can also enter the system through the boundaries according to the properties of an external source, e.g. an external radiation field. After entering the system a particle is followed along its trajectory through the mesh until it is absorbed at some point (r, t). If the particle encounters a scattering event, it will emerge with a new direction, energy and frequency as determined by the scattering law.

At census time, t^{n+1}, energies are tallied in each space zone $[r_j, \Delta r]$, and the properties of the radiation field are determined from the distribution of the particles. The balance of emission and absorption over the time step is calculated, and new material temperatures are obtained. The procedure is then repeated for each subsequent time step until the problem is terminated.

(a) *Source particle generation*

The number of source particles, N_j, to be emitted in each zone over a time step is arbitrary but must be judiciously controlled in order to minimize statistical fluctuations in the radiation field properties. The energies of the source particles are determined by dividing the total energy emitted over the time step in each zone equally among the N_j source particles assigned to the zone.

In addition to the energy E_p, the following characteristics must be assigned to each source particle emitted in zone j: point of emission (r_p, t_p) in the elementary rectangle $[r_j, \Delta r; t^n, \Delta t]$, direction cosine μ_p, frequency ν_p and distance to encounter S_{enc}, which may be either a scattering event or absorption. The values for S_{enc} must be assigned in such a way that encounters in a large group of particles occur exponentially

$$S_{\text{enc}} = \frac{1}{\sigma_t} \log \frac{1}{u_1}$$

where $\sigma_t = (\sigma_a + \sigma_s)$, and u is a random variable uniformly distributed in the interval (0, 1). After a particle travels a distance equal to S_{enc}, the event is absorption if

$$u_2 \leqslant \frac{\sigma_a}{\sigma_a + \sigma_s}$$

and scattering otherwise.

The values for r_p, t_p, μ_p, ν_p are distributed among the N_j source particles so as to reflect the appropriate properties of the emission function $\sigma_a^\nu B^\nu(T)$. In the simplest scheme, the emission function is considered uniform over the zone

and equal to the value at the zone center

$$r_p = r_j + u\,\Delta t$$

$$t_p = t^n + u\,\Delta t.$$

Since the emission is isotropic, the direction cosines are distributed uniformly in the interval $(-1, 1)$

$$\mu_p = 1 - 2u.$$

The frequencies are obtained from the emission function by a random sampling procedure [6]. A rejection process, although simple to construct, is not efficient; use of the cumulative probability distribution is efficient but difficult to construct in the case of cross-sections with lines and absorption edges.

(b) *Particle following*

After a particle enters the system it must be advanced through successive events until it either exits from the system, is absorbed, or reaches census at time t^{n+1}. Three distances along the particle path are required: the distance to the nearest zone boundary S_{bdy}, the distance to census S_{cen}, and the distance to encounter S_{enc}. If the particle crosses a zone boundary, S_{enc} must be modified to account for the resulting change in cross-section:

$$S'_{\text{enc}} = (S_{\text{enc}} - S_{\text{bdy}})\frac{\sigma_j}{\sigma_{j'}}.$$

If the particle reaches census, the coordinates r_p and μ_p are computed for census time t^{n+1} and stored together with E_p and ν_p for use on the next cycle. When a particle is absorbed or leaves the system, its history is ended.

(c) *Conservative scattering*

If a particle moving in the direction μ' encounters a scattering event, a new direction is chosen by random sampling from the scattering kernel $K(\mu, \mu')$. For isotropic scattering the new direction is independent of μ' and given by $\mu = 1 - 2u$. For Thompson scattering in the rest frame of the electron

$$K(\mu, \mu') = \tfrac{3}{16}[(3 - \mu^2) + (3\mu^2 - 1)(\mu')^2]$$

and the new direction is obtained by a rejection process. In conservative scattering the energy and frequency of the particle are left unchanged.

(d) *Radiation field properties*

The properties of the radiation field can be calculated in two different ways: by the *indicator* or counting method, and by the *expected value* method.

The indicated values for the frequency integrated energy density, flux, and radiation pressure are

$$E_{j+\frac{1}{2}} = \frac{1}{\Delta V_j}\sum_p \delta_p(j)E_p$$

$$F_{j+\frac{1}{2}} = \frac{c}{\Delta V_j}\sum_p \delta_p(j)\mu_p E_p$$

$$P_{j+\frac{1}{2}} = \frac{1}{\Delta V_j}\sum_p \delta_p(j)\mu_p^2 E_p$$

where $\delta_p(j) = 1$ if $r_j \leqslant r_p < r_{j+1}$, and $\delta_p(j) = 0$ otherwise. The expected values for these quantities are given by

$$E_{j+\frac{1}{2}} = \frac{1}{\Delta V_j}\sum_p \frac{S_p(j)}{c\,\Delta t}E_p$$

$$F_{j+\frac{1}{2}} = \frac{c}{\Delta V_j}\sum_p \frac{S_p(j)}{c\,\Delta t}\mu_p E_p$$

$$P_{j+\frac{1}{2}} = \frac{1}{\Delta V_j}\sum_p \frac{S_p(j)}{c\,\Delta t}\mu_p^2 E_p$$

where $S_p(j)$ is the distance travelled in zone j, by the particle p, on the time interval $[t^n, \Delta t]$.

The indicated value for the absorption in a zone is simply the sum of E_p for all particles absorbed in the zone on the time interval. The expected value for the total absorption in zone j over the interval is

$$\Delta E_{\text{abs}}(j) = \sum_p S_p(j)\,\sigma_a^{\nu_p} E_p.$$

In regions where the mean free path is much larger than $c\,\Delta t$ or Δx, the expected values for absorption show less statistical fluctuation than the indicated values. In regions of small mean free path, where most of the particles are absorbed, the indicated values are generally more accurate.

(e) *Temperature calculation*

The energy absorbed in each zone $\Delta E_{\text{abs}}(j)$ is obtained from the Monte Carlo calculation on the basis of the extrapolated temperature

$$T^*_{j+\frac{1}{2}} = T^n_{j+\frac{1}{2}} + \tfrac{1}{2}(T^n_{j+\frac{1}{2}} - T^{n-1}_{j+\frac{1}{2}})$$

which is assumed constant over the time step. The energy balance equation (2) is approximated by the difference form

$$\rho c_v T^{n+1}_{j+\frac{1}{2}} - \rho c_v T^n_{j+\frac{1}{2}} = \frac{\Delta E_{\text{abs}}(j)}{\Delta V_j} - c\,\Delta t \bar{\sigma}_p(T^{n+\frac{1}{2}}_{j+\frac{1}{2}})\, a(T^{n+\frac{1}{2}}_{j+\frac{1}{2}})^4.$$

The difference equation is solved in each zone for $T^{n+1}_{j+\frac{1}{2}}$ by Newton–Raphson iteration, assuming that

$$T^{n+\frac{1}{2}}_{j+\frac{1}{2}} = \tfrac{1}{2}(T^n_{j+\frac{1}{2}} + T^{n+1}_{j+\frac{1}{2}}).$$

It should be noted that in this treatment of the temperature equation the emission term $c\,\Delta t \bar{\sigma}_p a T^4$ is allowed to seek its own level in the iteration. Thus the equation is "buffered" with respect to statistical fluctuations which occur in the absorption term $\Delta E_{\text{abs}}/\Delta V$. As a result fluctuations in the temperatures are damped to a considerable extent, although energy is not conserved identically. The nonconservation of energy permits the use of this requirement as an important check on the accuracy of the calculation.

4. ACCURACY OF THE METHOD

There are two main sources of error in the Monte Carlo method: statistical error and truncation error. A measure of the accuracy of the calculation is given by the energy check, ϵ, where at any time

$$\epsilon = -1 + \frac{\text{(total radiation and material energy in the system)}}{\text{(total energy to enter the system)} - \text{(total energy to leave the system)}}.$$

Since ϵ exhibits considerable fluctuation in the course of the calculation, one is interested principally in $\bar{\epsilon}$, the time average, and $\pm\sqrt{[(\delta\epsilon)^2]}$, the mean square fluctuation.

Figures 1–4 illustrate the results of test problems designed to investigate the accuracy of the method. In each problem a plane, semi-infinite slab is heated by an external radiation field, $B^\nu(T_0)$. The slab is characterized by a constant absorption cross-section and constant specific heat.

(a) *Statistical error*

In Fig. 1 it can be seen that $\bar{\epsilon}$ approaches a lower limit as the total number of particles used at each time step in the calculation increases. The lower limit is set by the truncation error. In general, $\bar{\epsilon} \propto \sqrt{N}$ so that no substantial reduction in $\bar{\epsilon}$ can be achieved by using more than 4000 particles.

Consequently, it can be assumed that the average of ten runs of the same problem with different sets of random numbers and 4000 particles is very close to the true solution (apart from truncation error), and that the variance obtained from the ten runs represents the probable statistical error in any single 4000-particle run. Figure 2 reveals that the average of forty runs with different random numbers and 500 particles falls within the probable error of any single 4000-particle run. Therefore, it seems safe to conclude that, at least in this calculation, there is no propagation of statistical error.

(b) *Truncation error*

Figure 3 illustrates the dependence of $\bar{\epsilon}$ on the space, time zoning. The temperature equation is differenced such that the truncation error is quadratic in Δt. As Δr is reduced the statistical error increases, owing to a reduction in the number of particles per zone. Figure 4 shows the convergence of the Monte Carlo solution to a finite difference solution as Δr is reduced.

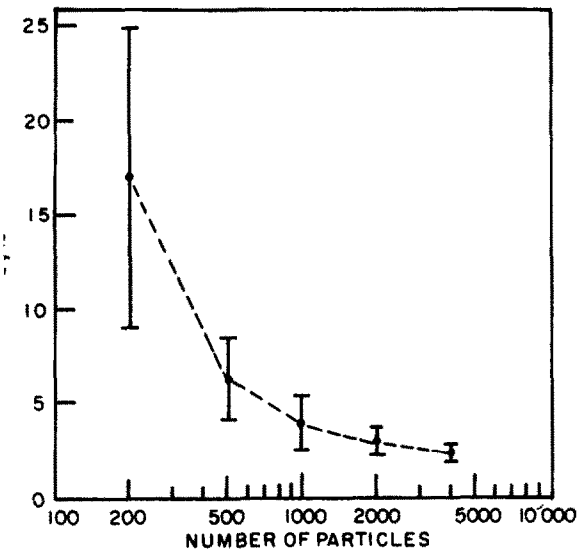

FIG. 1. Energy check, $\bar{\epsilon}$, as a function of the number of particles used in the calculation of a slab heating problem with constant mean free path ($\Delta x = c\,\Delta t = 0{\cdot}5\,\lambda$).

5. SAMPLE CALCULATION

To illustrate the Monte Carlo method in a frequency-dependent calculation, the following radiative heating problem is considered. A plane, semi-infinite slab of constant density and constant specific heat is exposed to an external radiation field, $B^{\nu}(T_0)$. The transport properties of the material are given by

$$\sigma_a^{\nu} = \sigma_0 \left(\frac{h\nu}{kT_0}\right)^{-3} \times \left[1 - \exp\left(-\frac{h\nu}{kT}\right)\right], \sigma_s = 0. \quad (5)$$

For this cross-section the Planck mean becomes

$$\bar{\sigma}_p(T) = \frac{15}{\pi^4}\,\sigma_0 \left(\frac{T}{T_0}\right)^{-3} \quad (6)$$

and the Rosseland mean is given to good approximation by

$$\bar{\lambda}_R \simeq \frac{15}{4\pi^4}\,7!\,\lambda_0 \left(\frac{T}{T_0}\right)^3. \quad (7)$$

The radiation and material energy densities in the slab are initially zero; it is necessary to obtain the distribution of these quantities as a function of time.

Figure 5 gives the distribution of temperature and radiant energy in a slab for gray-body

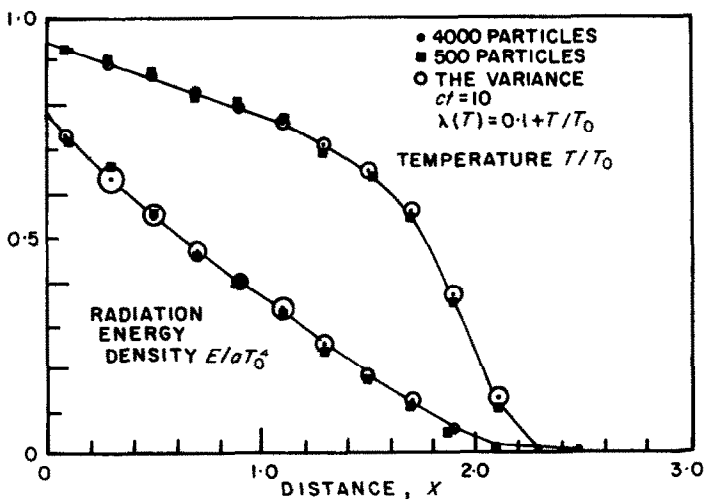

FIG. 2. Comparison of the average of ten 4000-particle runs with different sets of random numbers with the average of forty 500-particle runs with different random numbers ($\Delta x = c\,\Delta t = 0{\cdot}2$). Temperatures were calculated for the ideal gas equation of state with $\rho c_v = 0{\cdot}5917\,aT_0^3$.

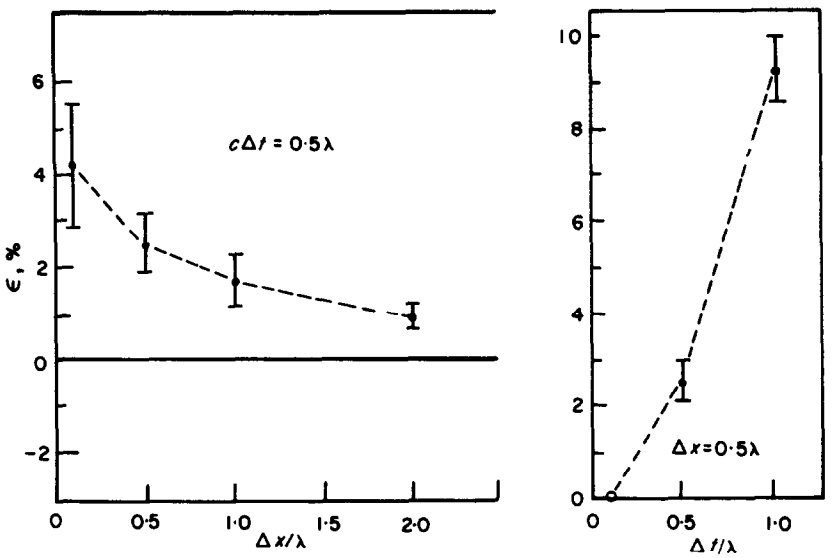

FIG. 3. Energy check, $\bar{\epsilon}$, as a function of the mesh size for a slab heating problem with constant mean free path. The calculations were performed with 400 particles.

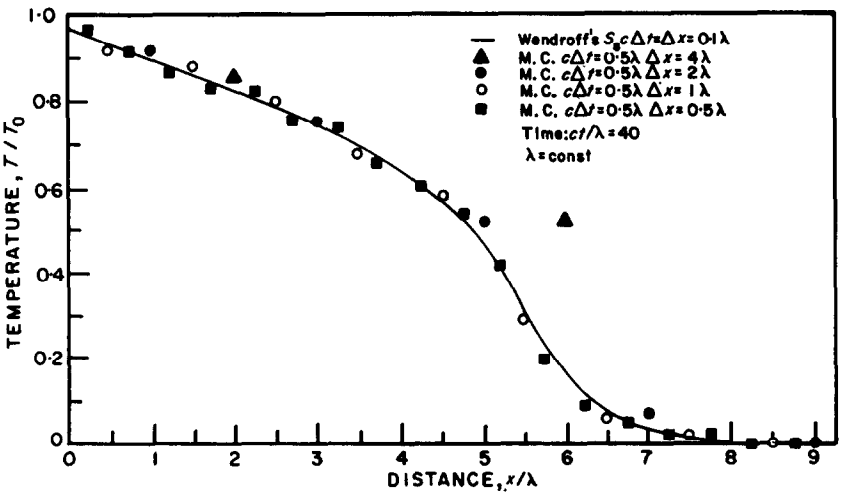

FIG. 4. Convergence of the Monte Carlo temperatures to the profile given by a finite difference solution. The finite difference solution is that given by Campbell [2], Fig. 1. Temperatures are for the ideal gas equation of state with $\rho c_v = 0.5917\, aT_0^3$. In each of the Monte Carlo calculations, 4000 particles were used.

transport using the Planck mean (6), for diffusion using the Rosseland mean (7) and for frequency-dependent transport using the cross-section (5).

All of the calculations were coded in FORTRAN and executed on the IBM-7094. The nonequilibrium diffusion calculation is that described by Campbell and Nelson [5]. In both of the Monte Carlo calculations 4000 particles were used with $c\,\Delta t = 2.5\,\lambda_0$, $\Delta x = 5\,\lambda_0$. The frequency-dependent calculation with expected values requires 1·5 s/c/thousand particles; a

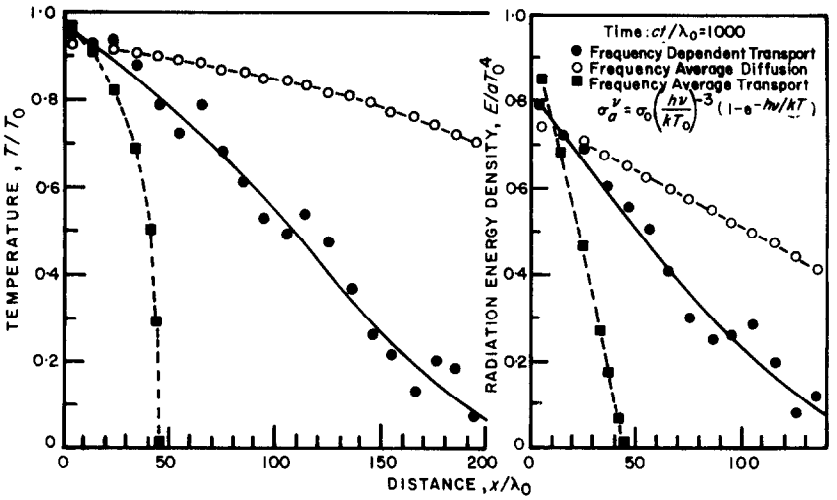

FIG. 5. Comparison of frequency-dependent transport with frequency-average transport using the Planck mean (6), and frequency-average diffusion using the Rosseland mean (7). Temperatures were obtained for the ideal gas equation of state with $\rho c_v = 0{\cdot}5917\ aT_0^3$.

total running time of 40 min for the problem of Fig. 5.

It is clear that the gray-body approximations are not at all appropriate for the solution of this problem. Agreement between a frequency-dependent calculation and a frequency-average calculation, which assigns a single mean free path to all particles in any small volume, can be expected only when the distance scale of the problem is large compared to the distribution of mean free path for the different frequencies present.

6. CONCLUSIONS

In this report a basic Monte Carlo method for nonlinear radiative transfer is described. Although the method has been illustrated here for only simple examples, it has been used successfully in many complex problems of a classified nature. The application to more realistic cross-sections and geometry requires little modification of the basic method.

The main advantage of Monte Carlo is that it directly simulates the physical process of particle transport; the application is straightforward (conceptually at least), and the correct physical behavior of the system is insured. The main disadvantage is that, in some problems, direct simulation of the physical process is an inefficient procedure for computation. For example, it is especially difficult to do diffusion or quasi-equilibrium calculations by Monte Carlo. In any region in equilibrium, the same energy that is emitted must be absorbed over a time step. Thus, the Monte Carlo temperatures are obtained from the difference of two large numbers, nearly equal, both of which contain statistical fluctuations.

Although Monte Carlo and finite difference calculations are comparable in terms of size, complexity and memory requirements, significant differences are found in accuracy and computing time. In Monte Carlo calculations, statistical error can be reduced by increasing the number of particles, and hence the running time. For this reason, it is difficult to give a meaningful comparison between the two methods except in specific examples. Campbell [2] solves the problem of Fig. 5 by a discrete ordinate method (with no statistical error) in somewhat less computing time than the Monte Carlo. In simple problems, such as that of Fig. 5,

finite difference methods generally have the advantage. In problems with material discontinuities at zone interfaces and complicated geometrical configurations, Monte Carlo has the advantage.

At present, there is no one method of numerical computation capable of handling all the radiative heating problems encountered in engineering applications. It is therefore advantageous to have both Monte Carlo and finite difference methods available for the solution of these problems.

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† UCRL Documents can be obtained from the clearing house for Federal Scientific and Technical Information, National Bureau of Standards, U.S. Dept. of Commerce, Springfield, Va.

Résumé—On décrit une méthode de Monte Carlo pour la solution numérique des problèmes non-linéaires du transport par rayonnement avec dépendance de la fréquence. La précision de la méthode est étudiée en tenant compte du nombre de particules nécessaires, de la propagation de l'erreur statistique, de l'erreur de troncature et de la convergence vers une solution connue.

On donne en exemple la solution d'un problème simple d'échauffement par rayonnement avec dépendance de la fréquence. Les calculs de corps gris employant à la fois le coefficient d'absorption moyen de Planck et le libre parcours moyen de Rosseland sont comparés avec le calcul avec dépendance de la fréquence.

Zusammenfassung—Eine Monte Carlo Methode zur numerischen Lösung nichtlinearer, frequenzabhängiger Strahlungsprobleme wird beschrieben. Die Genauigkeit der Methode wird untersucht im Hinblick auf die Zahl der erforderlichen Partikel, dem Fortschreiten des statischen Fehlers, des Abbruchfehlers und der Übereinstimmung mit einer bekannten Lösung. Die Lösung eines Problems der einfachen frequenzabhängigen Strahlungsheizung ist gezeigt. Berechnungen des grauen Körpers sowohl mit Hilfe des Plank'schen mittleren Absorptionskoeffizienten als auch der mittleren freien Weglänge nach Rosseland werden verglichen mit der frequenzabhängigen Berechnung.

Аннотация—Описан метод Монте Карло для численного решения нелинейных задач по лучистому теплообмену, зависящему от частоты. Точность метода исследовалась в зависимости от числа необходимых частиц, статистической погрешности, ошибки вследствие отбрасывания членов и сведения к известному решению. Дано решение простой задачи лучистого теплообмена, зависящего от частоты. Расчеты для серого тела, использующие средний коэффициент абсорбции Планка и среднюю длину свободного пробега Росселанда, сравниваются с расчетами лучистого теплообмена, зависящего от частоты.