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NON-LINEAR RADIATION TRANSPORT PROBLEMS INVOLVING WIDELY VARYING MEAN FREE PATHS

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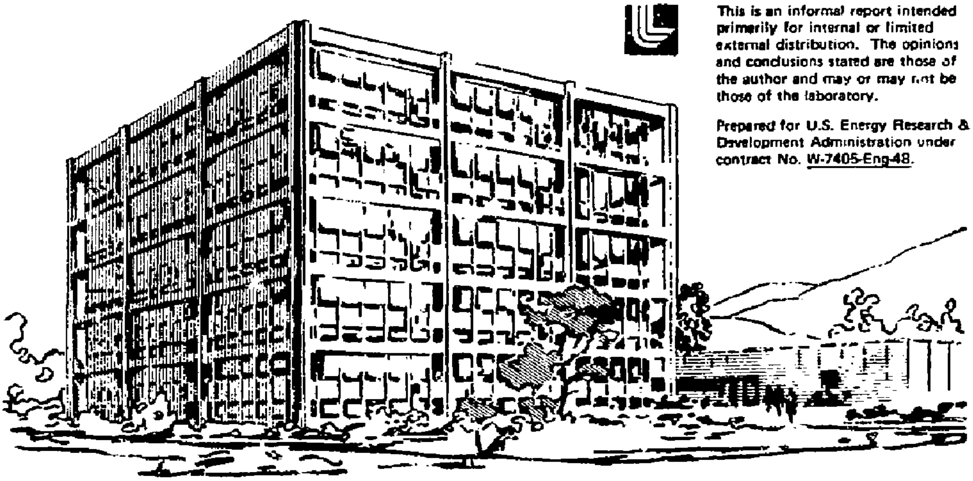

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I. INTRODUCTION

Although numerical methods have been developed for radiation transport problems in which either no very short mean free paths occur or only short mean free paths occur there exists no exact method for treating problems which involve both large and small mean free paths. When the number of mean free paths across a region is not too large at any frequency of interest then one may use the Monte Carlo method (1) to calculate the transport of radiation across the region. However, when the number of mean free paths across a region is large at some important frequencies then it may be inconvenient to use the Monte-Carlo method because of the long computation time needed. In this report a method will be given for modifying the Monte-Carlo approach so that one can accurately treat problems that involve both large and small mean free paths. This method purports to offer the advantages of the general Monte Carlo technique as far as relatively great accuracy of simulation of microscopic physical phenomena is concerned, and the advantage of a diffusion theory approach as far as decent time steps in thick problems are concerned; it does suffer from something of the statistical fluctuation problems of the Monte Carlo, although in analytically attenuated and modified form.

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Suppose we wish to compute the transport of radiation across a region where the mean free paths are small at all frequencies. Except for small transient effects the transport of radiation inside such a region can be calculated using the diffusion equation:

$$f = -D \frac{\partial e}{\partial x} \qquad (1)$$

where f is the flux of radiation, e is the radiation energy density, and D is the diffusion constant. The diffusion constant is related to the Rosseland mean free path λ by:

$$D = \frac{\lambda c}{3} \quad . \qquad (2)$$

The use of Eq. (1) is equivalent to assuming that the transport of radiation is due to the "random walk" of photons. Of course, a particular photon does not actually make a series of random steps but is instead absorbed after it has gone about a mean free path. However, when the mean free path is short the radiation is very nearly in equilibrium with the matter and so the rates of absorption and emission are balanced. Thus when a photon is absorbed another photon will be emitted in its place. Consequently, instead of explicitly following the emission and absorption of photons one can suppose that a photon merely changes direction after going a mean free path. If the radiation is in equilibrium with the matter at all frequencies then the radiation will have a Planck spectrum and so we need only to calculate the temperature. In fact for equilibrium radiation $e = aT^4$ so we can formulate the transport problem as a diffusion equation for the temperature (2).

Let us now ask how to treat the case where the mean free path is small at some frequencies but not all frequencies. The radiation in this case will not have a Planck spectrum and we must explicitly treat the radiation transport for each frequency. However, for those frequencies where the mean free path is small the rates of emission and absorption will after a short time be equal and so the transport of the photons at those frequencies can be described as a random walk. Thus, for those frequencies where the mean free path is small we can write:

$$f_\nu = -D_\nu \frac{\partial e_\nu}{\partial x} \tag{3}$$

where f_ν and e_ν are the flux and energy density at frequency ν and D_ν is related to the mean free path at frequency ν by $D_\nu = \lambda_\nu c/3$. This result suggests that transport problems involving widely varying mean free paths might be handled by using the Monte-Carlo method for photons with large mean free paths and diffusion theory for photons with small mean free paths. Of course, the mean free path can change greatly as a photon moves from one region to another or can change greatly as the temperature changes. Thus, one must be able to change from treating the transport of a photon via Monte-Carlo to using diffusion theory and visa versa. To put it another way we will in general need to match a Monte-Carlo "solution" for radiation transport with a solution of the diffusion equation. The solution of this matching problem is in fact the main difficulty confronting us. We will now show how this matching problem can be solved in an approximate fashion, thereby providing an approximate method for solving general radiation transport problems.

When a photon moves into a region where the mean free path is small it will of course be absorbed before it goes a few mean free paths. However, if the region is hot enough then we can suppose that the photon instead undergoes a series of scatterings. In this case as the photon enters the region its forward motion will be converted into a series of random steps in which it is equally likely to be moving in any direction. It still has some chance of moving forward but at a rate determined by diffusion theory. According to diffusion theory the distance which the photon can penetrate into the region in a time t is approximately given by:

$$d = \sqrt{2Dt} \qquad (4)$$

where D is the diffusion constant. This formula suggests that in order to match the Monte-Carlo solution for radiation transport to a solution of the diffusion equation we should slow the Monte-Carlo particles down so that Eq. (4) is satisfied. By slowing down the particles we will also slow down the rate of absorption which is in accord with the picture of particles undergoing a series of scatterings in a diffusing medium rather than being absorbed after going a few mean free paths. Of course, slowing down the Monte-Carlo particles according to Eq. (4) does not automatically guarantee that the correct rates for emission and absorption will be maintained or that the radiation energy will be transported at the correct rate.

For one thing, when photons are incident on a cold opaque region it would not be correct to slow down the rate of absorption of the photons. Thus we must increase the rate of absorption of slowing down particles to insure the correct rate of energy absorption in a cold medium. A little thought shows that we can insure the correct rate of energy absorption by demanding that the following equation be satisfied:

$$\frac{de_\nu}{dt} = -c\sigma_\nu(\tilde{e}_\nu - \frac{4\pi}{c} B_\nu) \qquad (5)$$

where σ_ν is the absorption cross-section (corrected for induced emission), B_ν is the Planck function, and $\tilde{e}_\nu$ is the "standing" energy density:

$$\tilde{e}_\nu \Delta\nu = \frac{1}{V} \sum_i \varepsilon_i \left(\frac{c-v_i}{c}\right) \qquad (6)$$

where ε_i and v_i are the energy and velocity of the i-th particle in the volume V and frequency interval $\Delta\nu$. The correction to the heating of the matter is obtained by taking the sum of the changes in $\tilde{e}_\nu$

$$\Delta E = \int_0^\infty d\nu \, \Delta \tilde{e}_\nu \qquad (7)$$

where E is the matter energy density. When the matter is out of equilibrium with the radiation at frequency ν, so that $\tilde{e}_\nu$ is smaller than $\frac{4\pi}{c} B_\nu$, then the matter will lose energy to the radiation and Eq. (5) will describe the rate of energy loss by the matter. We note that in a region with a small mean free path we will quickly arrive at a situation where $\tilde{e}_\nu = \frac{4\pi}{c} B_\nu$ in which case there will be no energy exchange between the radiation and matter.

Even apart from the question of energy absorption and emission, slowing down the particles according to Eq. (4) will in general not transport the radiation at the correct rate. In order to insure that radiation is transported across surfaces at the correct rate we must demand that the transport equation for radiation be satisfied. That is, we must demand that the radiation intensities $I_\nu(\Omega)$ satisfy

$$\frac{1}{c}\frac{\partial I_\nu}{\partial t} + \Omega \cdot \nabla I_\nu = c\sigma_\nu(I_\nu - \frac{1}{c} B_\nu) \quad . \tag{8}$$

Since the Monte-Carlo technique for particles transported at velcity c automatically guarantees that Eq. (8) is satisfied, the deviations from the correct rate of radiation are greatest for slow-moving particles. However, in a region where the particles are moving slowly the mean free path is small and therefore it should be sufficient to use Eq. (3) rather than the more complicated Eq. (8) to insure that radiation is transported at the correct rate. Actually it is not quite correct to use Eq. (3) because it involves the total energy density rather than the "standing" energy density. That is we should correct the radiation fluxes using the equation:

$$\Delta f_\nu = - \frac{\lambda_\nu c}{3} \frac{\partial \tilde{e}_\nu}{\partial x} \quad . \tag{9}$$

(there are situations where the flux would not be given by Eq. (9), e.g. a hot wall radiating into a vacuum. These situations can be approximately allowed for by using a frequency-dependent "flux limiter"). In order to insure that the slowing down particles satisfy Eq. (9) their motions will have to be modified. Essentially we will have to require that the motion of the particles is biased toward the forward or backward hemisphere enough to satisfy Eq. (9). A natural way to accomplish this is to pick out slow moving particles on a random basis and start them off again with velocity c in a direction chosen from either the forward or backward hemispheres, depending on the sign of the flux. In other words we should put in some real "scattering" to simulate the actual average random walk of a photon.

By slowing the Monte-Carlo particles down according to Eq. (4) and then demanding that Eqs. (5) and (9) be satisfied we will have in effect matched the Monte-Carlo "solution" of Eq. (8) with a solution of the diffusion equation. In regions where the mean free path is long we will be using the usual Monte-Carlo method while in regions where the mean free path is small we will be using the diffusion equation [Eq. (3)] to calculate the transport. When the mean free path changes from large to small (or visa versa) the method automatically switchs to using the appropriate approximation. Although our arguments have been somewhat heuristic we might point out that our matching method is analogous to matching techniques used in the theory of boundary layer flows (3). We now turn to a brief description of the actual numerical procedure.

II. THE NUMERICAL METHOD

We will consider one-dimensional problems involving a region of length L during a time T. The length L will be divided into a number of zones such that the material properties do not change greatly across a zone. The time T will be divided into a number of time steps such that the temperature does not change greatly in a time step. Energy bundles, or "particles", will be emitted in each space-time zone according to the rules given below. Particles can also enter the problem through the boundaries according to the properties of an external source. After emission a particle will move along a straight line with a velocity which decreases with distance according to the prescription given below. The particle will continue to move in a straight line until it is "scattered" or destroyed. At the end of each time step the amount of energy emitted and absorbed by each zone is computed. From the balance of emission and absorption the change in material temperature is computed. We now give the rules for each of the above operations.

Particle Emission. We replace the frequency interval $[o,\infty]$ by a set of frequency bins $[o,\nu_1]$, $[\nu_1,\nu_2]$, $\cdot\ \cdot\ \cdot$ $[\nu_{MAX-1},\nu_{MAX}]$}. We emit particles into each frequency bin with a uniform distribution in frequency within the bin. The energy to be emitted into a given frequency bin $[\nu_i, \nu_{i+1}]$ in a time step Δt is determined by integrating the right hand side of Eq. (5) over the frequency interval $[\nu_i, \nu_{i+1}]$:

$$\Delta e_\nu = \Delta t \int_{\nu_i}^{\nu_{i+1}} c\sigma_\nu \left(\frac{4\pi}{c} B_\nu - \tilde{e}_\nu \right) d_x \quad . \tag{10}$$

Here $\sigma_\nu(T)$ and $B_\nu(T)$ are calculated at the zone centers. The number of particles emitted into a frequency bin is determined from Δe_ν as follows: If Δe_ν is less than one-half the mean energy of the particles we don't emit any particles, if Δe_ν is greater than one-half the mean energy but less than twice the mean energy we emit one particle with energy Δe_ν, if Δe_ν is greater than twice the mean energy we emit as many particles as we can subject to the condition that each particle has the same energy and the energy of a particle is greater than the mean energy. The particles are emitted uniformly throughout the zone and time step. They are emitted in direction isotropically.

Particle Following. A particle enters the problem with a given energy, point or origin, time of origin, direction of emission, and frequency. A particle starts off with a velocity equal to the speed of light. As time goes on its velocity is decreased according to the following prescription. For the first zone that the particle is in the time it takes to go a distance s is $t_1(s)$:

$$\ell_1 t_1(s) = \frac{s^2}{c} \tag{11}$$

where ℓ_1 is the mean free path in the first zone. In the second zone the time it takes to go a distance s into the zone is determined by the equation

$$\ell_1 t_1(s_1) + \ell_2 t_2(s) = (s_1 + s)^2/c \tag{12}$$

where s_1 is the distance the particle traveled in the first zone and ℓ_2 is the mean free path in the second zone. In the k'th zone the time it takes to go a distance s into the zone is

$$\ell_k t_k(s) + \sum_{i=1}^{k-1} \ell_i t_i(s_i) = \left(s + \sum_{i=1}^{k-1} s_i\right)^2 / c \tag{13}$$

where s_i is the distance traveled in the ith zone and ℓ_i is the mean free path in the i-th zone. If a transit time t(s) derived from Eq. (13) turns out to be smaller than $\frac{s}{c}$ we set $t(s) = \frac{s}{c}$.

Energy Absorption. As a particle moves along we absorb energy from the particle according to the optical depth it has moved. If during a time step a particle moves a distance Δs in a zone with mean free path ℓ we deposit an amount of energy $E(1 - e^{-\Delta s/\ell})$, where E is the energy of the particle when it entered the zone.

Absorption Correction. In order to correct the absorption of energy for the slowing down of the particles we absorb an amount Δe_ν^a from the particles in a given zone and frequency bin. If $\frac{4\pi}{c}\bar{B}_\nu > \tilde{e}_\nu$ then $\Delta e_\nu^a = 0$. If $\tilde{e}_\nu > \frac{4\pi}{c}\bar{B}_\nu$ then Δe_ν^a is given by

$$\Delta e_\nu^a = \Delta t \int_{\nu_i}^{\nu_{i+1}} c\sigma_\nu (\tilde{e}_\nu - \frac{4\pi}{c} B_\nu)\, d\nu \quad . \tag{14}$$

The energy tax Δe_ν^a is distributed among the particles of the zone and frequency bin in proportion to each particles contribution to $\tilde{e}_\nu$.

Transport Correction. In order to insure that energy is moving across zone boundaries at the correct rate we use the following equation for the correction to the flux:

$$f_\nu = \frac{c}{3} \frac{\Delta\tilde{e}_\nu}{\left|\frac{1}{2}\left(\frac{\Delta x_1}{\ell_1} + \frac{\Delta x_2}{\ell_2}\right)\right| + \frac{4}{3}\left|\frac{\Delta\tilde{e}_\nu}{MAX\tilde{e}_\nu}\right|} \tag{15}$$

where Δx_1 and Δx_2 are the widths of the two zones and $\Delta\tilde{e}_\nu$ is the difference in the values of $\tilde{e}_\nu$ for the two zones. For each zone we compute two fluxes, flux f_ν^+ and f_ν^- corresponding to the two boundaries. If the sign of f_ν^+ corresponds to flow out of the zone we sweep thru the particles in the zone and choose particles to be "scattered" into the forward hemisphere by picking a random number $o \le u \le 1$ for each particle and then accepting the particle for scattering if

$$u \le \frac{c-v_i}{c} \frac{4f_\nu^+}{c\tilde{e}_\nu} \tag{16}$$

otherwise we reject the particle and leave it alone. "Scattering" consists of starting the particle out with velocity c in a direction randomly chosen in the forward hemisphere. A similar procedure is followed for the backward flux f_ν^-.

Temperature Calculation. The change in material temperature is calculated at the end of each time step by using the equation:

$$c_v(\bar{T})(T^{n+1} - T^n) = \Delta E_{abs} - \Delta e_\nu \qquad (17)$$

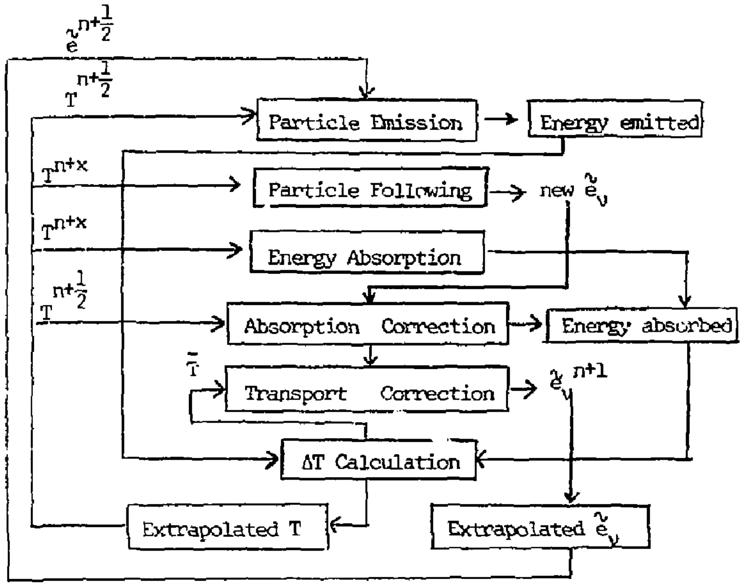
where ΔE_{abs} is the sum of the energy deposited directly from the particles and Δe_ν^a. This equation is solved for T^{n+1} by iteration assuming that

$$\bar{T} = \frac{1}{2}(T^{n+1} + T^n) \quad . \qquad (18)$$

The temperatures for the generation and following of particles and calculation of energy absorption are obtained by forward extrapolation

$$T^{n+1/2} = T^n + \frac{1}{2}(T^n - T^{n-1}) \quad . \qquad (19)$$

The sequence of operations in each time step is outlined in the following diagram



The temperature T^{n+x} denotes the temperature linearly extrapolated forward to the time when the particle enters a zone. The temperatures $\bar{T}$ and $T^{n+\frac{1}{2}}$ are defined in Eq.s (18) and (19). It should be noted that as far as transport is concerned our code is fully implicit.

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