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**IMPLICIT MONTE CARLO METHODS AND
NON-EQUILIBRIUM MARSHAK WAVE RADIATIVE TRANSPORT**

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ABSTRACT

Two enhancements to the Fleck implicit Monte Carlo method for radiative transport are described, for use in transparent and opaque media respectively. The first introduces a spectral mean cross section, which applies to pseudoscattering in transparent regions with a high frequency incident spectrum. The second provides a simple Monte Carlo random walk method for opaque regions, without the need for a supplementary diffusion equation formulation.

A time-dependent transport Marshak wave problem of radiative transfer, in which a non-equilibrium condition exists between the radiation and material energy fields, is then solved. These results are compared to published benchmark solutions and to new discrete ordinate S-N results, for both spatially integrated radiation-material energies versus time and to new spatially dependent temperature profiles. Multigroup opacities, which are independent of both temperature and frequency, are used in addition to a material specific heat which is proportional to the cube of the temperature.

TRANSPARENT MEDIUM SPECTRAL MEAN PSEUDOSCATTER CROSS SECTION

The very powerful implicit Monte Carlo photon transport method is quite well known. Some features are quickly reviewed here, preparatory to discussing a variation, based on Kirchhoff's law, which is sensitive to the actual spectrum in a transparent medium, for representing the pseudoscatter or reemission fraction. This fraction, with the companion absorption fraction, determines the net heating rate and equilibration time. If the usual assumption is adequate, that emission and reemission in a nearly transparent medium exactly obey the thermodynamic equilibrium theory, then this approach is identical to that based on the Kirchhoff-Planck relation. However, if that assumption is questioned, then this approach may be justified.

The radiation transport equation, in the absence of scattering, is:

$$1/c \partial I / \partial t + L(I) + \sigma_v I = \eta_v$$

where

$$\sigma_v = \rho \kappa_v(\rho, T)$$

including corrections for stimulated emission, and

$$I = I(\nu, \underline{\Omega}, t) .$$

The emission, if represented by Kirchhoff's law, is

$$\eta_v = \sigma_v I(\nu, \underline{\Omega}, t)$$

or by the usual Kirchhoff-Planck relation, is

$$\eta_v = c/4\pi \sigma_v B_v = \left(\frac{\sigma_v b_v}{4\pi \sigma_p} \right) c \sigma_p u_e$$

$$u_e = aT^4$$

which is strictly correct, only for a system in thermodynamic equilibrium. The term,

$$\left(\frac{\sigma_{\nu} b_{\nu}}{4\pi\sigma_p} \right)$$

represents both the frequency and directional dependence in the volume emission.

The LTE energy conservation equation is:

$$\partial u_m / \partial t = \int_0^{\infty} d\nu \oint_0^{\pi} d\Omega \sigma_{\nu} I - c/4\pi \int_0^{\infty} d\nu \oint_0^{\pi} d\Omega \sigma_{\nu} B_{\nu}$$

where

$$u_m = \rho c_{\nu} T .$$

As a variation on the original equilibrium definition of β_e ,

$$\partial u_r / \partial t = \beta_R \partial u_m / \partial t$$

where u_r is the true radiation energy density on the discretized time interval:

$$\Delta t = t^{n+1} - t^n$$

and

$$u_r = \alpha u_r^{n+1} + (1 - \alpha) u_r^n$$

with $\alpha = 1$ for a fully implicit solution.
It is obtained from:

$$u_r^{n+1} - u_r^n = \int_{t^n}^{t^{n+1}} dt \beta_R \left(\partial u_m / \partial t \right)$$

or

$$u_r^{n+1} - u_r^n = \int_{t^n}^{t^{n+1}} dt \left\{ \beta_R \int_0^{\infty} d\nu \oint_0^{\pi} d\Omega \sigma_{\nu} - \beta_R \bar{\sigma}_1 u_r^{n+1} \right\} ; \alpha = 1 .$$

This can be written as:

$$u_r^{n+1} - u_r^n = \Delta t \left[\beta_R \int_0^\infty dv \oint_0^{4\pi} d\Omega \sigma_v I - \beta_R \bar{\sigma}_I c u_r^{n+1} \right]$$

for appropriate average values of intensity, cross section and beta on the small time interval, Δt .

The equilibrium relationship between Kirchhoff's law and the Kirchhoff-Planck equation requires that:

$$\beta_e = \beta_R \bar{\sigma}_I / c_p$$

where

$$\bar{\sigma}_I = \frac{\int_0^\infty \sigma_v I_v dv}{\int_0^\infty I_v dv}.$$

This new β_R reduces to the original β_e at equilibrium, but serves to appropriately modify the pseudoscatter and absorption cross sections which are yet to be defined, in a transparent medium.

Finally:

$$u_r = u_r^{n+1} = \frac{(u_r^n + \Delta t \beta_R \int_0^\infty dv \oint_0^{4\pi} d\Omega \sigma_v I)}{(1 + \beta_R c \bar{\sigma}_I \Delta t)}$$

which can be inserted into the transport equation. This produces:

$$\begin{aligned} & 1/c \partial I / \partial t + L(1) + g \sigma_v I + (1 - g) \sigma_v I \\ & = \left(\frac{\sigma_v^b}{4\pi \sigma_p} \right) \left[g c \bar{\sigma}_I u_r^n + (1 - g) \int_0^\infty dv \oint_0^{4\pi} d\Omega \sigma_v I \right], \end{aligned}$$

where the g and $(1 - g)$ terms on the left side are absorption and out-pseudoscatter respectively, while the $(1 - g)$ term on the right side is in-pseudoscatter and the g term is volume emission. These positive fractions are defined to be:

$$f = \frac{1}{1 + \alpha \beta_e c \sigma_p \Delta t}$$

$$1 - g = \frac{\alpha \beta_R c \bar{\sigma}_I \Delta t}{1 + \alpha \beta_R c \bar{\sigma}_I \Delta t}$$

$$g = \frac{1}{1 + \alpha \beta_R c \bar{\sigma}_I \Delta t} ; \alpha = 1$$

The need to limit f to some arbitrary minimum value, such as 0.01, has now been eliminated insofar as pseudoscatter and absorption are concerned. The pseudoabsorption fraction, g , will be greater than f , until equilibrium is attained.

OPAQUE MEDIUM RANDOM WALK

The number of thick opaque Monte Carlo cells may be minimized by use of a hybrid Monte Carlo-diffusion method. Those opaque cells which remain in the Monte Carlo portion of a mesh may be treated by a diffusive particle random walk, under certain optical thickness and timestep constraints. The particle walk time interval is generally less than the total time remaining in a given Monte Carlo timestep, but must be sufficient to guarantee a minimum number of diffusive pseudocollisions, N , and thus obey the probability assumptions that depend on a large value for N . The maximum walk time interval, however, is also constrained, and N limited, so that the probability for a particle to cross a cell boundary during the walk is vanishingly small. The cell then is equivalent to an infinite medium, in this restricted walk time interval.

The spherical probability density function for final radial positions, R , after a large number of collisions, N , in an unbounded region is:

$$p_N(R) = \frac{e^{-(3|R|^2/2N\langle r^2 \rangle)}}{(2\pi N\langle r^2 \rangle/3)^{3/2}}$$

where $\langle r^2 \rangle$ is the mean square displacement between collisions.³

The normalized cumulative probability distribution function is then:

$$P_N(R) = \iiint d^3R p_N(R)$$

which results in

$$P_N(u) = \text{erf}(u) - \frac{2}{\sqrt{\pi}} u e^{-u^2}$$

where

$$u = R/(2N\langle r^2 \rangle/3)^{1/2}.$$

Since:

$$P_N(u = 3) \approx 1,$$

all particles remain within a spherical radius, for which $u \leq 3$. From reference 4,

$$N\langle r^2 \rangle = 2c\delta t\lambda_R$$

where δt is the particle walk time interval and λ_R is the Planck reciprocal mean pseudo cross section.

For a given spherical radius to the nearest cell boundary, R_b ,

$$u^2 = \frac{R_b^2}{(2*2c\delta t\lambda_R/3)}$$

and for $u = 3$, the maximum zig-zag travel distance during the walk time interval is therefore:

$$c\delta t_{\max} = \frac{R_b^2}{12\lambda_R}.$$

During this limited walk time interval, the cell is effectively infinite in extent and the new particle position may be randomly determined from the normalized probability distribution function for an unbounded region by a single table look-up, with:

$$\text{Random No.} = P_N(u),$$

which determines u , and therefore R .

If $c\delta t$ happens to be greater than that remaining in the Monte Carlo timestep, $c\Delta t$, the actual number of zig-zag segments is reduced to:

$$N = c\Delta t/\lambda_p$$

where λ_p is the Planck averaged pseudocollision mean free path.⁴ N must still be much greater than 1, if random walk is to occur. The actual u is randomly determined from $P_N(u)$, for thirty values of u from 0.0 to 3.0, with the random number on the interval 0.0 to 1.0.

The new particle position is then determined from:

$$R = u(4c\delta t\lambda_R/3)^{1/2},$$

where Δt is substituted for δt if necessary. The new direction cosines are determined from an isotropic distribution, as for a normal pseudoscatter in an unbounded medium.

NON-EQUILIBRIUM MARSHAK TRANSPORT WAVE

This problem is completely described in references 5-7. In this analysis, radiation from a constant isotropic source at 1 keV temperature is incident on a one-dimensional slab. The material specific heat is:

$$C_v(x, \tau) = \alpha/\rho T^3(x, \tau)$$

where

$$\epsilon = 16\sigma/c\alpha = 0.1$$

defines the constant α . Integrated non-dimensional radiation and material energies are obtained according to:

$$\psi(\tau) = \int_0^\infty dx (T(x, \tau)/T_H)^4$$

where T_H is the temperature of the constant source and $T(x, \tau)$ is either the material temperature or equivalent radiation temperature, defined by:

$$T_r^4(x, \tau) = I(x, \tau)/\sigma.$$

The optical depth is x , and the other non-dimensional independent variable is:

$$\tau = (\epsilon \kappa \rho) t .$$

Figure 1 displays the Monte Carlo results, which can be compared to the discrete ordinate S-N results in Figure 2, as well as the analytical results from reference 5. The agreement is quite good. Radiation and material temperatures versus depth in cm are shown in Figures 3 and 4, for both the Monte Carlo and discrete ordinate methods, for a single non-dimensional time. Again, the agreement is quite satisfactory.

Bradley Clark has contributed the S-N portion of this solution, and much essential collaboration in defining the problem. Robert E. H. Clark has provided new equation-of-state and opacity capabilities, for continued use in multigroup transport projects such as this.

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Figure 1. Monte Carlo Integrated Radiation and Material Energies for Marshak Transport Wave, with $\epsilon = 0.1$.

Figure 2. Discrete Ordinates S-N vs. Analytical Integrated Radiation and Material Energies for Marshak Transport Wave, with $\epsilon = 0.1$.

Figure 3. Monte Carlo vs. S-N Radiation Temperature (keV) vs. Depth (cm) for Marshak Transport Wave, with $\epsilon = 0.1$ and $\kappa\rho = 1.0$ at $\tau = 3.0$.

Figure 4. Monte Carlo vs S-N Material Temperature (keV) vs. Depth (cm) for Marshak Transport Wave, with $\epsilon = 0.1$ and $\kappa\rho = 1.0$ at $\tau = 3.0$.