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## An alternative Monte Carlo approach to the thermal radiative transfer problem

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#### ABSTRACT

The usual Monte Carlo approach to the thermal radiative transfer problem is to view Monte Carlo as a solution technique for the nonlinear thermal radiative transfer equations. The equations contain time derivatives which are approximated by introducing small time steps. An alternative approach avoids time steps by using Monte Carlo to directly sample the time at which the next event occurs. That is, the time is advanced on a natural event-by-event basis rather than by introducing an artificial time step.

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#### 1. Introduction

There are a number of methods for Monte Carlo solution of the thermal radiative transfer equations using discrete time steps; for example, see [1–3]. These discrete time steps are not really part of the thermal radiative transfer problem; they are an artifact of the way Monte Carlo is used to solve the thermal radiative transfer equations. The approach presented here advances the time on a natural event-by-event basis rather than by introducing an artificial time step.

Because there is no time step, the physical properties are not held fixed over a time step. Instead, the physical properties simply change on an event-by-event basis. If for example, there are N photons at time t and the next event is that the kth photon gets absorbed at t' > t, then the number of photons at time t' is N-1 and the energy of the kth photon is deposited in the material.

This event based approach will be illustrated a very simple infinite medium problem containing no scattering. Photons and the material are assumed to be in local thermodynamic equilibrium and the photon field and material exchange energy when the material absorbs or emits a photon.

It should be noted that there are many modeling approximations in real thermal radiative transfer problems. This paper introduces an alternative method that avoids the approximation associated with discretizing time. None of the other approximations (e.g. spatial discretization) is impacted. This paper basically assumes that everything is modeled as before, except for the time discretization. The paper shows how to remove the time discretization and model the time continuously.

The ideas presented may be worth considering for problems where the time discretization error is significant. It may be that for many problems the time discretization error is not a significant error source, in which case the Monte Carlo simulations will not be improved by the method discussed herein.

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This paper was written to describe an interesting alternative approach to simulating thermal radiative transfer developed by a person with no previous experience in the field. Practical applicability has neither been demonstrated nor claimed. Even if practical, the method may not prove competitive with existing methods that have been developed and proven their worth over several decades.

The paper is organized as follows:

- 1. Section 2 gives a very brief conceptual description of the thermal radiative transfer problem.
- 2. Section 3 defines terms and gives the radiative transfer equations.
- 3. Section 4 abstracts the physical process and directly builds a Monte Carlo process to simulate the physical process.
- 4. Sections 5 and 6 discuss frequency group approximations that focus on sampling rates rather than using time steps.
- 5. Sections 7 and 8 give results for a one group and a multigroup infinite medium problem.
- 6. Section 9 discusses the implications of having one computer particle represent many physical photons.
- 7. Section 10 gives some concluding comments.

#### 2. The thermal radiative transfer problem

This section gives a very brief conceptual description of the thermal radiative transfer problem. Note that a Monte Carlo model of the problem could be made at this point without ever mentioning any thermal radiative transfer equations. The physical process can be abstracted and a Monte Carlo process can be devised to simulate the physical process (see Section 4).

Note that a Monte Carlo process is typically far richer in information than the thermal radiative transfer equations. In fact, the thermal radiative transfer equations are one *particular* average over the Monte Carlo process. A Monte Carlo simulation can answer questions that the thermal radiative transfer equations cannot. For instance, what fraction of the particles entering region  $R_n$  were emitted in region  $R_i$  and then passed through regions  $R_j$ ,  $R_k$ ,  $R_l$ , and  $R_m$  before entering region  $R_n$ ? Perhaps such a question might be relevant in the design of some system, perhaps not, but a Monte Carlo simulation can easily answer such a question. Of course, one could write a *different* equation representing a different average over the Monte Carlo process. The point here is not to conflate a *particular* average over a random process with the random process itself.

Consider a small volume. The following events are possible:

- 1. A photon enters the volume through the boundary.
- 2. A photon is absorbed in the volume and the material temperature increases.
- 3. A photon is emitted by the material into the volume and the material temperature decreases.
- 4. A photon leaves the volume through the boundary.
- 5. A photon is emitted by an external source into the volume.

#### 3. The thermal radiative transfer equations

This section defines terms and gives the radiative transfer equations. Notwithstanding the comments in Section 2, these equations describe the averages that are typically desired. Apparently after displaying the radiative transfer equations, many Monte Carlo practitioners start viewing Monte Carlo as a way to solve the radiative transfer equations rather than as a way to model the thermal radiative transfer problem. Perhaps this is the reason for the near universal discretization of time in the codes. In essence, one abstracts the physical process, one averages over the physical process to obtain equations, and one then builds a Monte Carlo process to simulate the equations.

A few definitions are required before writing the thermal radiative transfer equations.

- 1. c = speed of light (300 cm/shake)
- 2.  $h = \text{Planck's constant} (4.132 \times 10^{-10} \text{ keV-shakes})$
- 3. t = time in shakes
- 4. v = frequency in cycles/shake
- 5.  $\Omega$  = direction
- 6.  $(\mathbf{r}, \mathbf{\Omega}, v, t)$  = (position, direction, frequency, time)
- 7.  $d\mathbf{r}$  = differential volume element in cm<sup>3</sup>
- 8.  $d\Omega$  = differential solid angle in steradians
- 9. dt = differential time interval in shakes
- 10.  $n(\mathbf{r}, \mathbf{\Omega}, v, t)d\mathbf{r} d\mathbf{\Omega} dv dt$  = number of photons in differential interval  $d\mathbf{r} d\mathbf{\Omega} dv dt$
- 11.  $I(\mathbf{r}, \Omega, v, t) = chvn(\mathbf{r}, \Omega, v, t)$  = specific intensity in units of keV/(cm<sup>2</sup>-steradian-shake-frequency interval)
- 12.  $T_K(\mathbf{r},t)$  = material temperature in degrees Kelvin (K)
- 13.  $k = 8.617343 \times 10^{-8} \text{ keV/K} = \text{Boltzmann's constant}$
- 14.  $T(\mathbf{r},t) = kT_k$  = material temperature in keV
- 15.  $B(v,T)dv = \frac{2hv^3}{c^2}(exp(hv/T) 1)^{-1}dv = \text{Planck's function for radiation (The number of photons emitted per shake in frequency interval } dv \text{ about } v \text{ from a material at temperature } T.)$

- 16.  $S(\mathbf{r}, \Omega, v, t) d\mathbf{r} d\Omega dv dt = \text{number of photons emitted in differential interval } d\mathbf{r} d\Omega dv dt$
- 17.  $Q(\mathbf{r}, \mathbf{\Omega}, v, t) = hvS(\mathbf{r}, \mathbf{\Omega}, v, t)d\mathbf{r} d\mathbf{\Omega} dv dt = \text{energy emitted in differential interval } d\mathbf{r} d\mathbf{\Omega} dv dt$
- 18.  $c_{\nu}(\mathbf{r}, T)$  = specific heat of material in keV/K
- 19.  $\sigma_a(\mathbf{r}, v, T)$  = absorption probability per cm (opacity)

With these definitions, the radiative transfer equations can be written [4]

$$\frac{1}{c} \frac{\partial I(\mathbf{r}, \mathbf{\Omega}, \mathbf{v}, t)}{\partial t} + \mathbf{\Omega} \cdot \nabla I(\mathbf{r}, \mathbf{\Omega}, \mathbf{v}, t) + \sigma_a(\mathbf{r}, \mathbf{v}, T)I(\mathbf{r}, \mathbf{\Omega}, \mathbf{v}, t) = \sigma_a(\mathbf{r}, \mathbf{v}, T)B(\mathbf{v}, T) + Q(\mathbf{r}, \mathbf{\Omega}, \mathbf{v}, t)$$
(1)

$$c_{\nu}(\mathbf{r},T)\frac{\partial T(\mathbf{r},t)}{\partial t} = \int_{0}^{4\pi} \int_{0}^{\infty} \sigma_{a}(\mathbf{r},\nu',T)(I(\mathbf{r},\Omega',\nu',t) - B(\nu',T))d\Omega'd\nu'$$
(2)

For this paper it will be more convenient to use the particle density  $n(\mathbf{r}, \mathbf{\Omega}, v, t)$  rather than the specific intensity  $I(\mathbf{r}, \mathbf{\Omega}, v, t)$ . The radiative transfer equations can then be written as

$$\frac{\partial n(\mathbf{r}, \mathbf{\Omega}, \mathbf{v}, t)}{\partial t} = -c\mathbf{\Omega} \cdot \nabla n(\mathbf{r}, \mathbf{\Omega}, \mathbf{v}, t) - \sigma_a(\mathbf{r}, \mathbf{v}, T)cn(\mathbf{r}, \mathbf{\Omega}, \mathbf{v}, t) + \sigma_a(\mathbf{r}, \mathbf{v}, T) \frac{B(\mathbf{v}, T)}{h\mathbf{v}} + S(\mathbf{r}, \mathbf{\Omega}, \mathbf{v}, t)$$
(3)

$$\frac{\partial T(\mathbf{r},t)}{\partial t} = \frac{1}{c_{\nu}(\mathbf{r},T)} \int_{0}^{4\pi} \int_{0}^{\infty} (\sigma_{a}(\mathbf{r},\nu',T)ch\nu'n(\mathbf{r},\Omega',\nu',t) - \sigma_{a}(\mathbf{r},\nu',T)B(\nu',T))d\Omega'd\nu'$$
(4)

#### 4. A Monte Carlo view of a very simple radiative transfer problem

This section shows that if one views the Monte Carlo process as modeling the physical process, then time discretization does not naturally appear. The time discretization appears to be an artifact of viewing the Monte Carlo process as solving an equation rather than modeling the physical process. In essence, one abstracts the physical process and directly builds a Monte Carlo process to simulate the physical process.

Consider a small volume. The number of photons in the volume change by photons moving in or out of the volume, photons getting absorbed in the volume, photons being emitted into the volume from the heated material, and external photon sources.

For simplicity, consider a problem with reflective spatial boundary conditions without any external sources (Q = S = 0). Suppose that there are N photons in the volume with frequencies  $v_i$  for i equal 1 to N. For this special problem there is no dependence on  $\mathbf{r}$  or  $\Omega$ . There is no flow in or out of the volume because of the reflective boundary conditions. One of two things can happen to change the temperature T (see Eq. (4); a particle is absorbed or a particle is emitted. Note that  $\sigma_a(v_i, T)$  is the interaction probability per unit distance traveled for photon i at frequency  $v_i$ . In a time dt the photon moves a distance c dt, so that the probability of interaction in time dt for photon i is  $\sigma_a(v_i, T)c$  dt. The interaction rate for photon i is thus  $\sigma_a(v_i, T)c$ . Summing over all photons (and noting that there is no scattering) gives the total absorption rate. Adding in the Planck emission rate gives the total rate  $R_T$  at which either a photon is absorbed or a photon is emitted:

$$R_T = \sum_{i=1}^{N} c\sigma_a(v_i, T) + V \int_0^\infty 4\pi c\sigma_a(v, T) \frac{B(v, T)}{hv} dv$$
 (5)

That is,  $R_T dt$  is the probability that the next event occurs in dt. The time to the next event is sampled from

$$p(t)dt = exp(-R_Tt)R_T dt$$

where  $exp(-R_Tt)$  is the probability that nothing happens before time t and  $R_T dt$  is the probability that an event occurs in the next dt after t.

An absorption is the next event with probability

$$p_{a} = \frac{\sum_{i=1}^{N} c\sigma_{a}(v_{i}, T)}{\sum_{i=1}^{N} c\sigma_{a}(v_{i}, T) + V \int_{0}^{\infty} 4\pi c\sigma_{a}(v, T) \frac{B(v, T)}{hv} dv}$$
(6)

An emission is the next event with probability

$$p_{e} = \frac{V \int_{0}^{\infty} 4\pi c \sigma_{a}(v, T) \frac{B(v, T)}{hv} dv}{\sum_{i=1}^{N} c \sigma_{a}(v_{i}, T) + V \int_{0}^{\infty} 4\pi c \sigma_{a}(v, T) \frac{B(v, T)}{hv} dv}$$
(7)

If an absorption is the next event, then photon k is the absorbed photon with probability

$$p_{ak} = \frac{\sigma_a(\nu_k, T)}{\sum_{i=1}^{N} c \sigma_a(\nu_i, T)}$$
(8)

In this case, the kth photon disappears and its energy,  $hv_k$  is deposited in the volume V causing the temperature to increase by

$$\Delta T = \frac{h v_k}{C_n(T) V} \tag{9}$$

If an emission is the next event, then photon N+1 is emitted with v sampled in dv about v with probability

$$p_{emit}(v)dv = \frac{4\pi c\sigma_{a}(v,T)\frac{B(v,T)}{hv}dv}{\int_{0}^{\infty} 4\pi c\sigma_{a}(v',T)\frac{B(v',T)}{hv'}dv'}$$
(10)

In this case, the new photon's energy,  $hv_{N+1}$ , is removed from the material in the volume V causing the temperature to decrease by

$$\Delta T = -\frac{h\nu_{N+1}}{c_{\nu}(T)V} \tag{11}$$

The Monte Carlo process for this problem is

- 1. Start with an initial temperature  $T = T_0$  and an initial number of photons  $N = N_0$  at frequencies  $v_i$ .
- 2. Compute the rate  $R_T$  from Eq. (5).
- 3. Sample the time  $t_{ne}$  to the next event using the rate  $R_T$  and update to the new time  $t \leftarrow t + t_{ne}$ .
- 4. Sample between emission or absorption using probabilities from Eqs. (6) and (7).
- 5. If an absorption occurs, go to step 7. If an emission occurs, go to step 6.
- 6. Emission occurs
  - a. Sample the emitted  $v_{N+1}$  from Eq. (10).
  - b. Update the number of photons to  $N \leftarrow N + 1$ .
  - c. Decrease the temperature per Eq. (11).
  - d. Recalculate opacities,  $\sigma_a(v_i, T)$ , for all photons i = 1, 2, ..., N at the new T. (Note  $\sigma_a(v_i, T)$  is not the same for all photons because the photons have different frequencies  $v_i$ .)
  - e. Output information on time, temperature, and photons for this event time.
  - f. Go to step 2.
- 7. Absorption occurs
  - a. Sample which photon was absorbed via Eq. (8).
  - b. Update the number of photons to  $N \leftarrow N 1$ .
  - c. Increase the temperature per Eq. (9).
  - d. Recalculate opacities,  $\sigma_a(v_i, T)$ , for all particles i = 1, 2, ..., N at the new T. (Note  $\sigma_a(v_i, T)$  is not the same for all photons because the photons have different frequencies  $v_i$ .)
  - e. Output information on time, temperature, and photons for this event time.
  - f. Go to step 2.

This approach is based on sampling rates rather than solving an equation with a time derivative. A few observations are worthwhile emphasizing.

- 1. There is no artificial  $\Delta t$  time step.
- 2. No approximations of constant properties in  $\Delta t$ .
- 3. Temperature changes only by emission or absorption.
- 4. Properties (e.g. opacities and temperature) are updated at sampled events.

#### 5. Multigroup radiative transfer equations

Define a group energy  $E_g$  in terms of a group frequency  $v_g$ 

$$E_{\sigma} = h \nu_{\sigma} \tag{12}$$

(Note that  $v_i$  has already been used for the *i*th particle's frequency so a different symbol has been used for the frequency of group g.) The multigroup form of Eqs. (3) and (4) is

$$\frac{\partial n_g(\mathbf{r}, \mathbf{\Omega}, t)}{\partial t} = -c\mathbf{\Omega} \cdot \nabla n_g(\mathbf{r}, \mathbf{\Omega}, t) - \sigma_{ag}(\mathbf{r}, T)cn_g(\mathbf{r}, \mathbf{\Omega}, t) + \sigma_{ag}(\mathbf{r}, T)\frac{B_g(T)}{h\nu_g} + S_g(\mathbf{r}, \mathbf{\Omega}, t)$$
(13)

$$\frac{\partial T(\mathbf{r},t)}{\partial t} = \frac{1}{c_v(\mathbf{r},T)} \sum_{g=1}^{G} \int \left( \sigma_{ag}(\mathbf{r},T) c E_g n_g(\mathbf{r},\Omega',t) - \sigma_{ag}(\mathbf{r},T) B_g(T) \right) d\Omega'$$
(14)

#### 6. Source-Free infinite medium multigroup equations

Consider a spatial volume V for which the particle density is independent of  $\mathbf{r}$  and  $\Omega$ . (This might happen, for example, if V has reflective boundary conditions.) In this case, the spatial gradient term in Eq. (13) is zero. Now integrating Eqs. (13) and (14) over  $\mathbf{r}$  and  $\Omega$  and defining

$$N_g(t) = V \int_0^{4\pi} n_g(\mathbf{r}, \mathbf{\Omega}, t) d\mathbf{\Omega}$$
 (15)

yields

$$\frac{dN_g}{dt} = \sigma_{ag}(4\pi V B_g / E_g - c N_g) \tag{16}$$

$$\frac{dT}{dt} = \frac{1}{c_v V} \sum_{g=1}^G \sigma_{ag} (cE_g N_g - 4\pi B_g)$$
 (17)

Consider the problem from a particle perspective as in Section 4. Let *N* be the number of particles. Again, there is no flow in or out of the volume because of the reflective boundary conditions. One of two things can happen to change *T*; a particle is absorbed or a particle is emitted. Let

$$\sigma_i$$
 = the opacity ( $\sigma_{ag}$ ) for the ith particle (18)

The rate at which the *i*th particle collides is  $c\sigma_i$ . The rate at which one of the *N* particles collides is

$$\sum_{i=1}^{N} c\sigma_i \tag{19}$$

The rate at which the material emits a particle is

$$V\sum_{g=1}^{G}\sigma_{ag}4\pi B_{g}/E_{g} \tag{20}$$

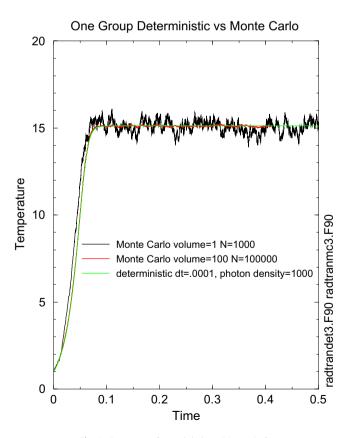


Fig. 1. One group deterministic vs Monte Carlo.

The total rate  $R_T$  at which something happens is:

$$R_{T} = \sum_{i=1}^{N} c\sigma_{i} + V \sum_{g=1}^{G} \sigma_{ag} 4\pi B_{g} / E_{g}$$
 (21)

The probability that the next event is absorption is

$$p_{a} = \frac{\sum_{i=1}^{N} c\sigma_{i}}{\sum_{i=1}^{N} c\sigma_{i} + V \sum_{g=1}^{G} \sigma_{ag} 4\pi B_{g} / E_{g}}$$
(22)

The probability that the next event is an emission is

$$p_{e} = \frac{V \sum_{g=1}^{G} \sigma_{ag} 4\pi B_{g} / E_{g}}{\sum_{i=1}^{N} c \sigma_{i} + V \sum_{g=1}^{G} \sigma_{ag} 4\pi B_{g} / E_{g}}$$
(23)

If the next event is an absorption, the kth photon is absorbed with probability

$$p_k = \frac{\sigma_k}{\sum_{i=1}^N c\sigma_i} \tag{24}$$

#### 7. One group results

For a single group, the g subscripts on  $E_g$  in Section 6 are superfluous and are dropped. For example,  $E = E_1$ . Using this notation, the radiative transfer equations can be written

$$B_1 = \int_0^\infty B(\nu, T) d\nu = \frac{ac}{4\pi} T^4$$
 (25)

$$\frac{dN}{dt} = \sigma_a(acVT^4/E - cN) \tag{26}$$

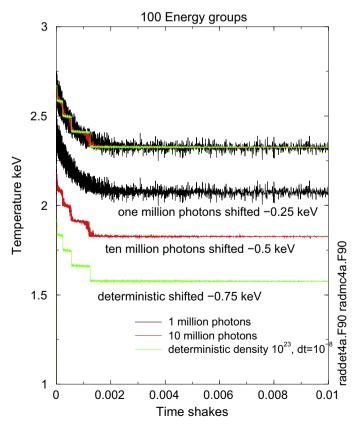


Fig. 2. 100 Energy groups. Particles start at 24.875 keV.

$$\frac{dT}{dt} = \frac{1}{c_{v}V}\sigma_a(cEN - acVT^4) \tag{27}$$

$$a = 0.01372$$
 (28)

$$\sigma_a = T$$
 (29)

$$c = 1 \tag{30}$$

$$c_v = 20 \tag{31}$$

$$E=1 (32)$$

$$N(0) = 1000 \text{ V}$$
 (33)

$$T(0) = 1 \tag{34}$$

Simple deterministic and Monte Carlo computer programs were written so that the Monte Carlo method could be compared against deterministic results. The problem is a source free infinite medium problem described by the parameters in Eqs. (28)–(34). The Monte Carlo procedure was described in Section 4. The deterministic code solved Eqs. (26) and (27) using a time step  $\Delta t$  of 0.0001 and an initial photon density of 1000. That is,

$$\Delta N = \sigma_a (acVT^4/E - cN)\Delta t$$

$$\Delta T = \frac{1}{c_n V} \sigma_a (cEN - acVT^4) \Delta t$$

Fig. 1 shows that with only 1000 photons the Monte Carlo results match the deterministic results fairly well, but with lots of statistical noise. In contrast, when 100,000 photons are used, the Monte Carlo results are very close to the deterministic results.

#### 8. 100 group results

This section compares deterministic and Monte Carlo results for a 100 energy and 100 temperature group problem. The Planck function is only sampled at the midpoint temperatures of the temperature groups. This temperature discretization

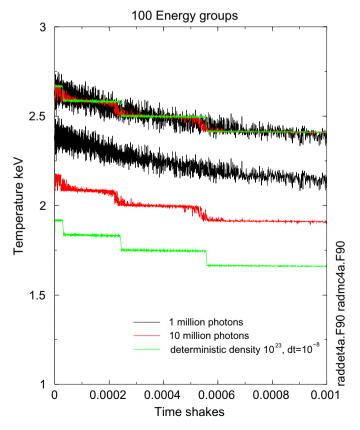


Fig. 3. 100 Energy groups. Particles start at 24.875 keV.

was done to avoid building extensive tables necessary to enable the sampling in Eq. (10) for continuous temperature. (Experienced radiative transfer experts may know good ways to do this, but the author does not.) The main objective is to demonstrate that the proposed method works on energy dependent problems as well as energy independent problems. There are some small unphysical artifacts associated with the temperature discretization, but the artifacts match between deterministic and Monte Carlo calculations.

Simple deterministic and Monte Carlo computer programs were written so that the Monte Carlo method could be compared against deterministic results. The group variables were determined using center values and interval widths. Specifically

$$E_{max} = 25 \text{ keV} \tag{35}$$

$$\Delta E = E_{max}/100 = 0.25 \text{ keV}$$
 (36)

$$E_{g} = \left(g - \frac{1}{2}\right)\Delta E \tag{37}$$

$$T_{max} = 8.6717343 \text{ keV}$$
 (38)

$$\Delta T = T_{max}/100 = 0.086717343 \text{ keV}$$
 (39)

$$T_i = \left(i - \frac{1}{2}\right) \Delta T \tag{40}$$

$$B_{gi} = B(E_g/h, T_i)\Delta E \tag{41}$$

$$\sigma_{ag} = T + E_g/5 \tag{42}$$

The specific form for the opacity was chosen simply to show that the method can easily treat a simultaneous dependence on energy and temperature; there is no physical reason for the particular dependence chosen.

Note that  $\sigma_{ag}$  changes with each absorption and emission because temperature does. This means that when a photon gets absorbed or emitted then the opacity values for all N photons in the problem change.

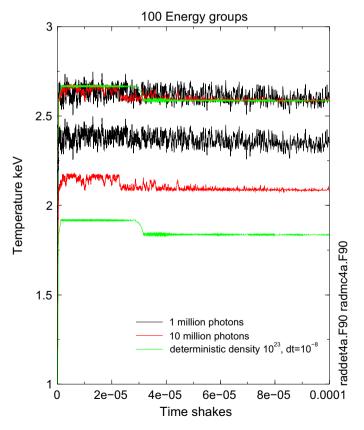


Fig. 4. 100 Energy groups. Particles start at 24.875 keV.

When the material is cold, and absorption dominates, the number of absorptions is proportional to the number of photons, say N. But on each absorption the temperature changes, so that there are N-1 opacities that change. Thus the number of opacity lookups scales like  $N^2$  for cold absorption dominated regimes, unless a little cleverness is used. When the material is hot, and emission dominates, the number of opacity lookups will be N times the number of emissions, unless a little cleverness is used.

Note that  $\sigma_{ag}$  does not change too much on an individual event. Keeping the number of opacity lookups under control was done via the standard Monte Carlo "delta scatter" [5–7] trick. This trick uses a fictitious opacity  $\sigma_{fict} > \sigma_a$  that is larger than the real opacity. The time sampling is done with the fictitious opacity and then when a collision occurs the collision is accepted with probability  $\sigma_a/\sigma_{fict}$ . If the collision is not accepted, then the photon "delta scatters" keeping the same precollision properties and the temperature is not changed. With delta scattering, one only needs to look up the true opacity for the particular photon that is colliding, rather than N opacity lookups.

Note that even with "delta scatter," only one photon is absorbed or emitted at a time and the temperature is still incremented or decremented one photon at a time. The statistical properties of the calculation are identical with or without "delta scatter." Delta scattering merely saves time.

Figs. 2–6 show deterministic and Monte Carlo results for the 100 group problem with an initial photon density of  $1 \times 10^{23}$  (all in the highest energy group) and an initial temperature of T = 1 keV. The reference deterministic calculation used a time step of  $1 \times 10^{-8}$  shakes. Two Monte Carlo calculations were done, one started with one million initial particles and one with ten million particles. Fig. 2 shows the approach to equilibrium. Initially, the material is cold and emission is low compared to absorption. The distribution of photons in the top energy group is very non-Planckian and the material must absorb these photons and redistribute them according to Planck's distribution This causes the temperature to rise rapidly to about 2.7 keV, as shown in Figs. 5 and 6. Once the supply of high energy photons starts to get depleted, the absorbed photons are then of lower energy. The material then starts emitting more energy than it is absorbing, and the temperature drops.

One question that has arisen concerning the 1 million particle and 10 million particle results in Figs. 2–6 is why bother displaying both? Note that for linear Monte Carlo transport codes where the particles are independent, if  $N_1$  particles give total score of  $S_1$  and  $N_2$  particles give a total score of  $S_2$ , then  $N_1 + N_2$  particles give a total score of  $S_1 + S_2$ . The expectations are also preserved so that if the entire calculation were repeated M times then  $\langle S_1 + S_2 \rangle_M = \langle S_1 \rangle_M + \langle S_2 \rangle_M$ . The thermal radiative transfer problem, however, is a nonlinear problem and the photons interact through the temperature dependence of the

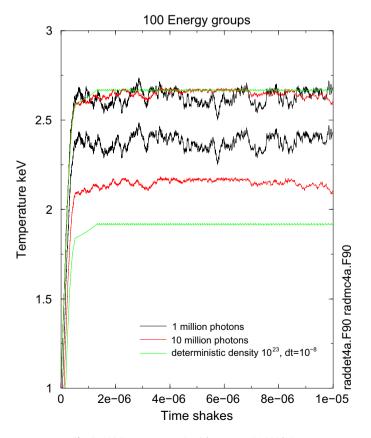


Fig. 5. 100 Energy groups. Particles start at 24.875 keV.

opacities and Planck distribution. As the number of photons gets large, photon i is impacted less and less by what happens to photon j. That is, photons i and j start to look independent. By contrast, if there are only two photons, then what happens to photon i has a significant dependence on what happens to photon j. This dependence can introduce a systematic bias in the calculation. Comparing the 1 million and 10 million results in Figs. 2–6, gives confidence that 1 million is large enough that there is essentially no systematic bias discernable.

The Monte Carlo results are noisy and lie on top of the deterministic results. To show the shape of the results better, a shifted version of the same results is shown also. The rapid changes in temperature in both the deterministic and Monte Carlo results are probably due to the discrete Planck function changing discontinuously between temperature ranges. For example, see the temperature behavior with 100 and 1000 temperature groups in Fig. 7. The ten million photon Monte Carlo results exhibit the rapid changes, but the statistical noise in the one million photon Monte Carlo results obscures the steps.

#### 9. Implications of one computer particle representing many photons

The new approach is exact when the number of computer photons is the same as the number of photons in the physics model. In practice, the physics model may have such a large number of photons that it is impractical to have one computer photon for each photon in the model. The new approach can easily be made to work with one computer photon representing *M* photons in the model, but then the approach is no longer exact because the random walks of the *M* photons are then sampled together rather than independently as in the physics model. Three points are worth noting:

- 1. Most, probably all, other Monte Carlo methods also represent *M* photons in the model by one computer photon with weight *M*. Thus the new approach is not introducing any new approximation.
- 2. The traditional approaches have a time discretization error in addition to the error associated with sampling *M* photons together. For practical problems with large numbers of computer photons, the time discretization error is probably by far the larger of the two errors. (This speculation has not been investigated.) The new approach has no time discretization error.

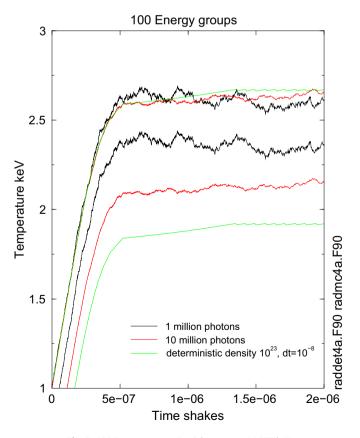


Fig. 6. 100 Energy groups. Particles start at 24.875 keV.

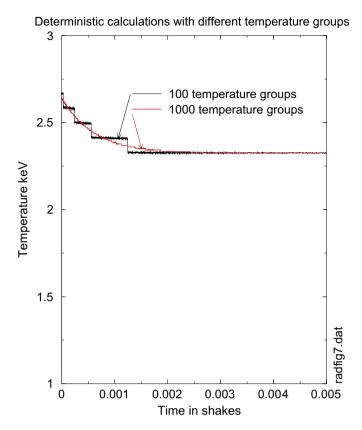


Fig. 7. Deterministic calculations with different temperature groups.

3. If desired, correlated sampling techniques can be used to estimate the difference between having done a calculation with each computer photon representing M model photons and each computer photon representing, say K = M/2, model photons.

#### 10. Conclusion

This paper has shown an alternative method to solve some thermal radiative transfer problems. The method recognizes that a "time step" is not part of the thermal radiative transfer problem. Instead, the "time step" in traditional methods (e.g. implicit Monte Carlo) is part of the numerical differencing of the thermal radiative transfer equations. The method presented here avoids the time step by using Monte Carlo to simulate the problem directly rather than simulating differenced equations.

A number of comments are worthwhile about the new method:

- 1. This alternative approach avoids an artificial "time step"; time changes solely based on events. This eliminates errors associated with approximating physical properties over a "time step".
- 2. The method is "exact" when the number of computer photons equals the number of physical photons. In practice, this means that the method is "exact" only as *N* gets infinite. (The results so far do not indicate problems for finite *N*.) Traditional Monte Carlo methods also have this approximation, so it is not a new approximation.
- 3. The method substitutes standard Monte Carlo tricks (e.g. delta scattering) for standard numerical tricks like a time step and implicit differencing schemes.
- 4. This work shows that this alternative approach is doable in principle, but it is not clear whether the approach will be competitive in practice.
- 5. The problem is complex and probably will require clever tricks, whether one uses Monte Carlo to solve the problem directly, or whether one uses Monte Carlo to solve the radiative transfer equations with a time step.
- 6. This alternative approach is a bit closer to the physics, so with luck, any approximations necessary to solve practical problems will be more driven by physics considerations than driven by numerical analysis considerations.
- 7. No claims are being made about the practical utility and/or competitiveness of the new method with existing methods. The author hopes to investigate these questions later, as time permits, with expert colleagues in this field.

#### References

- [1] C. Ahrens, E.W. Larsen, A 'Semi-analog' Monte Carlo method for grey radiative transfer problems, in: Proceedings of the American Nuclear Society Mathematics and Computations Topical Meeting, Salt Lake City, Utah, September 2001.
- [2] L.L. Carter, C.A. Forest, Nonlinear radiation transport simulation with an implicit Monte Carlo method, Los Alamos report LA-5038, Los Alamos National Laboratory, 1973.
- [3] J.A. Fleck Jr., J.D. Cummings, An implicit Monte Carlo scheme for calculating time and frequency dependent radiation transport, J. Comput. Phys. 8 (1971) 313.
- [4] Gerald.C. Pomraning, The Equations of Radiation Hydrodynamics, Dover Publications, Inc., Mineola, New York, 1973. Permagon Press ISBN 0-08-016893-0.
- [5] E.R. Woodcock, T. Murphy, P.J. Hemmings, T.C. Longworth, Techniques used in the GEM code for Monte Carlo neutronics calculations in reactors and other systems of complex geometry, in: Proc. Conf. Applications of Computing Methods to Reactor Problems, ANL- 7050, Argonne National Laboratory, 1965, p. 557.
- [6] L.L. Carter, E.D. Cashwell, W.M. Taylor, Monte Carlo Sampling with Continuously Varying Cross Sections Along Flight Paths, Nucl. Sci. Eng. 48 (1972) 403–411.
- [7] S.N. Cramer, Application of the Fictitious Scattering Radiation Transport Model for Deep- Penetration Monte Carlo Calculations, ORNL/TM-4880, Oak Ridge National Laboratory, 1977.