



LAWRENCE
LIVERMORE
NATIONAL
LABORATORY

A Modified Treatment of Sources in Implicit Monte Carlo Radiation Transport

N. A. Gentile, T. J. Trahan

March 29, 2011

22nd International Conference on Transport Theory
Portland, OR, United States
September 11, 2011 through September 15, 2011

Disclaimer

This document was prepared as an account of work sponsored by an agency of the United States government. Neither the United States government nor Lawrence Livermore National Security, LLC, nor any of their employees makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States government or Lawrence Livermore National Security, LLC. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States government or Lawrence Livermore National Security, LLC, and shall not be used for advertising or product endorsement purposes.

A MODIFIED TREATMENT OF SOURCES IN IMPLICIT MONTE CARLO RADIATION TRANSPORT

N. A. Gentile

Lawrence Livermore National Laboratory L-38
 7000 East Avenue
 Livermore, CA 94551
 gentile1@llnl.gov

Travis J. Trahan

Department of Nuclear Engineering & Radiological Sciences
 University of Michigan
 1928 Cooley Building
 2355 Bonisteel Boulevard
 Ann Arbor, Michigan USA 48109-2104
 tjtrahan@umich.edu

We describe a modification of the treatment of photon sources in the IMC algorithm [1]. We describe this modified algorithm in the context of thermal emission in an infinite medium test problem at equilibrium and show that it completely eliminates statistical noise.

Let us examine the case of an infinite medium problem with gray, constant opacities with matter and radiation at equilibrium at temperature T , simulated with the IMC method. The census photons representing the initial radiation all initially have time $t = 0$ and have a total energy aT^4 . During a time step of size Δt , the energy of each census photon will decrease by a factor $\exp[-\sigma c \Delta t]$. The total energy in census photons at the end of the time step will therefore be

$$E_{census}(t = \Delta t) = aT^4 \exp[-\sigma c \Delta t]. \quad (1)$$

To simulate thermal emission, we will make N_s thermal source photons, each with a different initial time $t_{i,p}$ in $[0, \Delta t]$. We will assume all N_s photons have the same initial energy $a c \sigma_P T_0^4 V \Delta t / N_s$. Since $t_{i,p}$ is different for each thermal source photon, they will all reach time Δt with different energies $E_p(t = \Delta t) = E_p(t = 0) \exp[-\sigma c (\Delta t - t_{i,p})]$. The sum of these energies will be

$$E_{thermal} \equiv \sum_{p=1}^{N_s} E_p(t = \Delta t) = aT_0^4 V c \sigma \Delta t \frac{1}{N_s} \sum_{p=1}^{N_s} \exp[-\sigma c (\Delta t - t_{i,p})]. \quad (2)$$

Since

$$\lim_{N_s \rightarrow \infty} \frac{1}{N_s} \sum_{p=1}^{N_s} \exp[-\sigma c (\Delta t - t_{i,p})] = \frac{1}{\Delta t} \int_0^{\Delta t} \exp[-\sigma c (\Delta t - \tau)] d\tau = \frac{1 - \exp[-\sigma c \Delta t]}{\sigma c}, \quad (3)$$

the sum in Eq.(2) is a Monte Carlo estimate for an integral over all possible thermal emission times. Using Eq.(2) and Eq.(3), we find that, in the limit of a large N_s , the radiation energy due to thermally emitted

photons at $t = \Delta t$ will be

$$E_{thermal}(t = \Delta t) = aT_0^4V(1 - \exp[-c\sigma\Delta t]), \quad (4)$$

so $E_{census} + E_{thermal} = aT_0^4V$, which is the value necessary to maintain thermal equilibrium. The matter energy will also be the same as the initial value, by energy conservation. With a finite number of photons, we will not maintain thermal equilibrium exactly, because the sum in Eq.(2) will only approximate the integral, with an error that is proportional to $N_s^{-\frac{1}{2}}$ [2].

This is illustrated in Fig. 1. This plot shows an IMC simulation using one zone, a cube with unit length in each direction. All faces have reflecting boundaries, making it effectively an infinite medium problem. The material and radiation temperatures were initialized to 1. The material has a heat capacity $c_v = 1.0$, and an absorption opacity $\sigma = 10$. The simulation used 100 photons per time step, and units were chosen so that $a = c = 1$. The simulation used $\Delta t = 0.001$ from $t = 0$ to $t = 1$, $\Delta t = 0.01$ from $t = 1$ to $t = 2$, and $\Delta t = 0.1$ for $t > 2$.

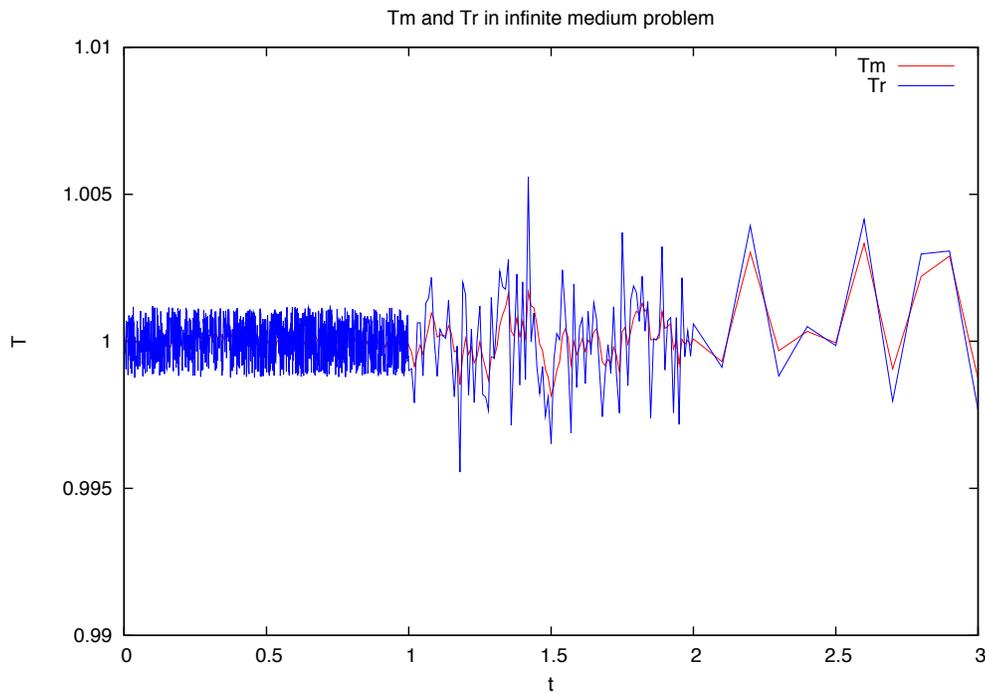


Figure 1. Matter and radiation temperature for an infinite medium test problem simulated with IMC with three different values for the time step Δt .

In the IMC algorithm, we regard physical quantities like opacity and heat capacity as constant throughout the time step. This means that the distance to scatter, the amount of absorption on a given photon path, etc.,

are independent of when they occur during the time step. We can therefore calculate the contribution that is made for every emission time in $[t^n, t^{n+1}]$ for each path taken by a source photon. This modified IMC algorithm is best illustrated by describing how we simulate the behavior of a source photon. As in IMC, we sample a position, direction, frequency, and energy E_p for each source photon. However, we do not sample an emission time. The energy emitted in a small period $[t_e, t_e + dt]$ will be $dE = \frac{E_p}{\Delta t} dt$. So we can think of a source photon as a large number of small photons with emission times spread out evenly between t^n to t^{n+1} , each with energy dE . Instead of the source photon having a time, it will have a distance traveled, s_p , with an initial value of 0. The photon will travel a total distance $c\Delta t$ in the time step, unless it exits the problem through a boundary. Some fraction of its energy will reach census on each path, and some fraction will be absorbed. These fractions will be functions of the initial and final value of s_p on the path. The total energy $E_p(s_p = 0)$ of the source photon will be either absorbed, leave the problem through a boundary, or reach census as the photon reaches $s_p = c\Delta t$. That is, $E_p(s_p = c\Delta t) = 0$.

First, we will calculate the amount of energy that reaches census on a given path from s_0 to $s_1 = s_0 + d_p$. Because of absorption, $dE(s_0 + d_p) = dE(s_0)[1 - \exp(-\sigma_a d_p)]$. The energy emitted in $[t^{n+1} - s_0/c, t^{n+1} - s_1/c]$ will reach census during the path. A photon that has moved a distance s_0 has a total energy consisting of emission that occurred in $[t^n, t^{n+1} - s_0/c]$. This range has a size of $t^{n+1} - s_0/c - t^n = \Delta t - s_0/c$, so

$$dE(s_0) = \frac{E_p(s_0)}{[\Delta t - s_0/c]} \quad (5)$$

and

$$dE(s) = dE(s_0)\exp[-\sigma(s - s_0)]. \quad (6)$$

The total energy reaching census is the integral of Eq.(6) over the range $[s_0, s_1]$:

$$E_c(s_0, s_1) = \int_{s_0}^{s_1} dE(s) = \frac{E_p(s_0)}{[\Delta t - s_0/c]} \int_{s_0}^{s_1} \exp[-\sigma(s - s_0)] = \frac{E_p(s_0)}{\sigma[\Delta t - s_0/c]} [1 - \exp[-\sigma(s_1 - s_0)]]. \quad (7)$$

Next, we will calculate the amount of energy that is absorbed on the path from s_0 to s_1 . This is done by conservation of energy. The photon energy at s_1 is related to the photon energy at s_0 by

$$E_a(s_0, s_1) + E_c(s_0, s_1) + E_p(s_1) = E_p(s_0). \quad (8)$$

$E_p(s_1)$ in Eq.(8) is given by Eq.(5). This yields

$$E_a(s_0, s_1) = E_p(s_0)(1 - \exp[-\sigma(s_1 - s_0)]) \frac{\Delta t - s_1/c}{\Delta t - s_0/c} - E_c(s_0, s_1). \quad (9)$$

The modified IMC results for the test problem described earlier are show in Fig. 2

Fig. 2 shows that there is no statistical noise in the modified IMC simulation for any value of Δt . This happens because the source photons in the modified IMC algorithm each contribute exactly the amount of

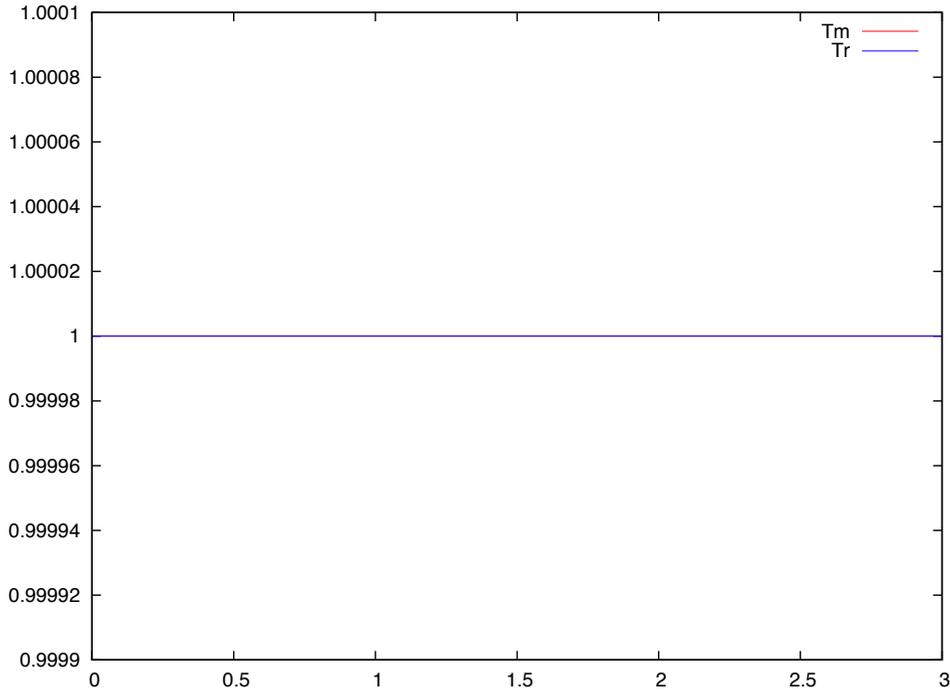


Figure 2. Matter and radiation temperature for infinite medium test problem using modified IMC with three different time steps

energy calculated in Eq.(2) to census. In effect, the integrand in Eq.(3) is evaluated exactly, not approximately as a sum over a finite number of emission times. The value of T_r at the end of the time step is 1.0 to roundoff. By conservation of energy, $T_m = 1.0$ to roundoff at the end of the time step also, and so these values are maintained in subsequent time steps of the calculation.

ACKNOWLEDGMENTS

The work of the first author performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

REFERENCES

- [1] J. A. Fleck, Jr., and J. D. Cummings, “An Implicit Monte Carlo Scheme for Calculating Time and Frequency Dependent Nonlinear Radiation Transport,” *J. Comput. Phys.*, **8**, pp. 313-342 (1971).
- [2] M. A. Kalos and P. A. Whitlock, *Monte Carlo Methods, Second Edition*, Wiley-VCH, Weinheim Germany. (2008).