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Smoothed Emission for IMC

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Smoothed Emission for IMC

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1. The current source algorithm for IMC

Here is a review of the current way we handle source photons in IMC.

A source photon is created with a randomly sampled position x_p in the zone, a direction Ω_p , a frequency ν_p sampled from the appropriate distribution, and a time t_p uniformly sampled from $[t^n, t^{n+1}]$. The source photons each have an energy E_p . The sum of E_p over all of the photons equals the energy of the source for that time step. In the case of thermal emission in a zone with volume V , we would have

$$\sum_{p=1}^N E_p = \sigma_P a c T^4 V \Delta t, \quad (1)$$

where N is the number of thermal source photons for that time step, and σ_P is the Planck mean opacity.

Census photons do not differ from source photons in any way, except that they all start the time step with $t_p = t^n$.

Then we advance each photon until it reaches the end of the time step. This advance consists of 4 steps.

Step 1 of this process is to calculate the following quantities: the distance to the zone boundary $d_b(x_p, \Omega_p)$; the distance to scatter $d_s = -\ln(r)/\sigma_s$, where r is a random number uniform in $[0, 1]$; and the distance to census $d_c = t^{n+1} - t_p$. We take the minimum of these 3 distances: $d_p = \text{Min}(d_b, d_s, d_c)$.

Step 2 is to advance the photon a distance d_p . We change the photon's position $x_p \rightarrow x_p + \Omega_p d_p$, the photon time to $t_p + d_p/c$, and remove an amount of energy $E_p[1 - \exp(-\sigma_a d_p)]$ from the photon. This energy is added into the material, because it represents absorption.

Step 3 is to simulate the physical activity that was supposed to occur at the distance d_p . For example, if $d_p = d_s$, we would do a scatter, which would result in a change of Ω_p . If $d_p = d_b$, we move the photon to a new zone. If $d_p = d_c$, we are through advancing the photon in this time step.

Step 4 is to go back to step 1, unless the photon we are advancing has reached census. Since we keep increasing t_p , the photon will eventually reach census, and the process will terminate.

When we are done with all of the photons, we update the matter temperature using the difference between the emitted and absorbed energy, and proceed to the next time step.

Let's look at applying this process to one time step of a problem in thermal equilibrium, where the matter temperature T_m = the radiation temperature $T_r = T_0$. To simplify things, we'll have one zone with volume V and reflecting boundaries, so that we are simulating an infinite medium. To further simplify, we will assume that σ is independent of frequency.

We start the simulation with an initial set of N_c photons, each with $t_p = 0$ and initial energies satisfying

$$\sum_{p=1}^{N_c} E_p(t=0) = a T_0^4 V. \quad (2)$$

These photons represent the initial radiation energy in the problem. Each of these photons will be advanced in time from $t = 0$ to $t = \Delta t$, and each will travel a distance $c \Delta t$. So each photon will reach Δt with an energy $E_p(t = \Delta t) = E_p(t = 0) \exp(-\sigma c \Delta t)$. So the radiation energy density due to the census photons at the end of the time step will be

$$E_{r,census} = \sum_{p=1}^{N_c} E_p(t = \Delta t)$$

2

$$\begin{aligned}
&= \sum_{p=1}^{N_c} E_p(t=0) \exp(-\sigma c \Delta t) \\
&= aT_0^4 V \exp(-\sigma c \Delta t).
\end{aligned} \tag{3}$$

To simulate thermal emission, we will make N_s thermal source photons, each with a different initial time $t_{i,p}$, with energies that satisfy

$$\sum_{p=1}^{N_s} E_p(t=0) = ac\sigma_P T_0^4 V \Delta t. \tag{4}$$

We will make the energy of all the thermal source particles equal, so for these particles $E_p(t = t_{i,p}) = ac\sigma_P T_0^4 V \Delta t / N_s$.

Each thermal source photon will move from the time it is created until the end of the time step. 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

$$\begin{aligned}
\sum_{p=1}^{N_s} E_p(t = \Delta t) &= \sum_{p=1}^{N_s} E_p(t=0) \exp[-\sigma c(\Delta t - t_{i,p})] \\
&= aT_0^4 V c \sigma \Delta t \frac{1}{N_s} \sum_{p=1}^{N_s} \exp[-\sigma c(\Delta t - t_{i,p})]
\end{aligned} \tag{5}$$

where we have used the assumption that all thermal photons had the same initial energy.

In the limit $N_s \rightarrow \infty$,

$$\frac{1}{N_s} \sum_{p=1}^{N_s} \exp[-\sigma c(\Delta t - t_{i,p})] \rightarrow \frac{1}{\Delta t} \int_0^{\Delta t} \exp[-\sigma c(\Delta t - \tau)] d\tau. \tag{6}$$

In other words, the sum in Eq.(5) is a Monte Carlo estimate for an integral over all possible thermal emission times. The integral in Eq.(6) can be performed analytically:

$$\int_0^{\Delta t} \exp[-\sigma c(\Delta t - \tau)] d\tau = \frac{1 - \exp[-c\sigma \Delta t]}{c\sigma}. \tag{7}$$

Using this expression, we find that, in the limit of a large number of particles, the radiation energy due to thermally emitted photons at $t = \Delta t$ will be

$$aE_{r,thermal} = aT_0^4 V (1 - \exp[-c\sigma \Delta t]), \tag{8}$$

and the sum of $E_{r,census}$ given in Eq.(3), and $E_{r,thermal}$ will be $aT_0^4 V$, 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, because the sum in Eq.(5) will only approximate the integral.

The important point is that, for this infinite medium problem, even with a finite number of particles, the census photons will give exactly the right value for their contribution to the radiation

energy, but the thermally emitted photons will not. This happens because the emission is sampled at discrete times, so the contribution to the radiation energy density at the end of the time step from the thermal photons is only approximate.

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 $t > 2$.

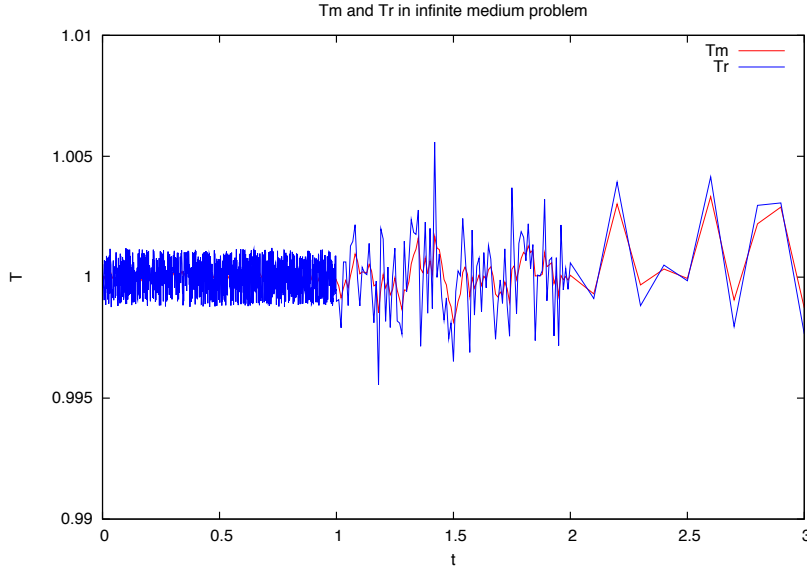


Figure 1: Matter and radiation temperature for infinite medium test problem using IMC with three different time steps

Fig. 1 shows the statistical noise in the IMC simulation. The noise increases with Δt . This happens because the integrand in Eq.(6) changes value more when Δt is large - the exponential decay of the energy of the thermal photons is larger over a larger time step. When the integrand varies more, a Monte Carlo approximation, like the sum in Eq.(6) has a larger variance, so the statistical noise increases.

As noted above, the noise in the simulation is caused by the choice of emission times for the thermally emitted photons. If we could eliminate the statistical noise caused by the choice of the emission time, then the matter and radiation temperature in Fig. 1 would be exactly 1 at all times, independent of Δt .

This is illustrated further in Figs. 2 and 3. These plots show the results of simulations that are the same as that in Fig. 1, except that the problem does not begin in equilibrium and Δt is

fixed at 0.001.

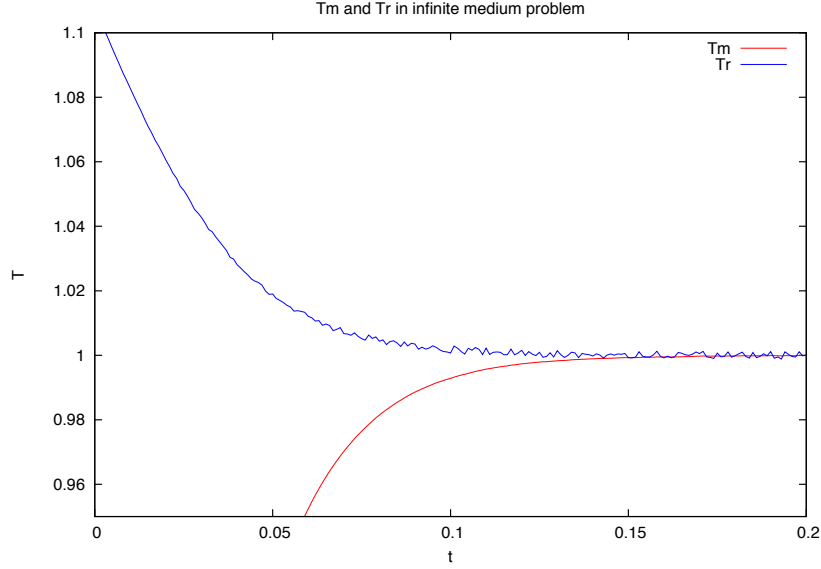


Figure 2: Matter and radiation temperature using IMC for infinite medium test problem with $T_r > T_m$ initially.

In the simulation in Fig. 2, the initial radiation temperature was higher than the initial matter temperature. Because of the low initial matter temperature, there is less thermal emission at the beginning of the problem than at late times, and the radiation energy density at early times is dominated by the initial census photons. As T_m becomes closer to T_r , photons created by thermal emission become more important. Fig. 2 shows that the radiation temperature is less noisy at early times, and becomes noisy when T_m becomes closer to T_r .

In Fig. 3, we show the results of a simulation in which T_m is initially much larger than T_r . In this simulation, thermally emitted photons are always important, and the radiation temperature shows statistical noise even at early times.

The results of the simulations shown in Figs. 2 and 3 are consistent with the idea that the thermal photons, because of the statistical noise created by the selection of their emission times, are the source of statistical noise in infinite medium Monte Carlo simulations.

We have only considered infinite medium problems in this section. In a simulation with multiple zones, we would also see statistical noise from the random choice of position and direction of both the thermally emitted photons and the census photons. So eliminating the noise from the sampling of emission times would not eliminate all statistical noise in more complicated simulations. However, some simulations with opaque zones with small time steps can have zones where most of the thermally emitted photons are absorbed before leaving the zone. These simulations could conceivably show a reduction of statistical noise if the sampling of the time of thermal

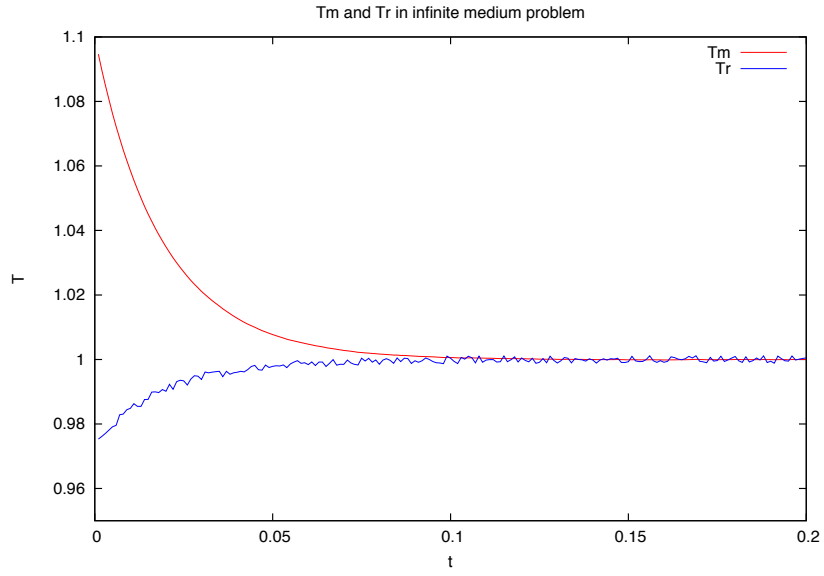


Figure 3: Matter and radiation temperature using IMC for infinite medium test problem with $T_m > T_r$ initially.

emission was made more accurate.

In the next section, we will discuss a way to eliminate the statistical noise due to the sampling of emission time.

2. The speculative new source algorithm for IMC

In the last section, we established that the statistical noise due to the choice of the emission time of thermal source photons caused the noise in the temperature of infinite medium problems. In this section, we will show how to eliminate this noise.

In the IMC algorithm, we regard physical quantities like opacity and heat capacity as constant throughout the time step. This means that quantities like the distance to scatter, and the amount of absorption on a given photon path are independent of the time during the time step. We can take advantage of this fact to calculate the contribution that is made for every emission time between t^n and t^{n+1} for each path taken by a source photon. We will refer to this as the modified IMC algorithm in the remainder of this document. Census photons, which have a definite time (specifically, the beginning of the time step, t^n), are treated in exactly the same as in standard IMC.

The modified IMC algorithm is best illustrated by describing how we simulate the behavior of a source photon. As in the standard IMC algorithm, we sample a position x_p , a direction Ω_p , and a frequency ν_p . The energy of the source photon, E_p is also sampled in the same way as standard IMC. However, we do not sample an emission time for the photon. Instead, we will regard the energy as being “spread out” over the whole time step, from t^n to t^{n+1} . The energy emitted in a small period $[t_e, t_e + dt]$ will be $dE = \frac{E_p}{\Delta t} dt$. So in the modified IMC algorithm, we can think of a source photon with a definite emission time and energy E_p as being replaced by a large number of small sub-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 that we update as it travels, we will keep track of how far it travels, which we will denote by s_p . The initial value of s_p is 0. During the whole time step, it will travel a total distance $c\Delta t$, unless it exits the problem through a boundary.

Since the modified IMC source photon does not have a time, it does not reach census in the traditional way. 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 $E_p(s = 0)$ 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. We will characterize the path as extending from s_0 to $s_1 = s_0 + d_p$. Since the absorption opacity is constant during the time step, the energy emitted in a small time period $[t_e, t_e + dt]$ (which we can think of as one of our sub-photons) will change to $dE(s_0 + d_p) = dE(s_0)[1 - \exp(-\sigma_a d_p)]$, independent of the value of t_e , on a path of length d_p . The sub-photons born between $t^{n+1} - s_0/c$ and $t^{n+1} - s_1/c$ will reach census during the path, and we want to know the sum of their energies.

When the photon has moved a distance s_0 , the total energy that our photon has consists of emission that occurred for t_e in the range $[t^n, t^{n+1} - s_0/c]$. This range has a size of $t^{n+1} - s_0/c - t^n = \Delta t - s_0/c$, so

$$dE(s_0) = \frac{E_p(s_0)}{[\Delta t - s_0/c]} \quad (9)$$

and

$$dE(s) = dE(s_0)\exp[-\sigma(s - s_0)]. \quad (10)$$

The total energy reaching census is the integral of Eq.(10 over the range $[s_0, s_1]$:

$$E_c(s_0, s_1) = \int_{s_0}^{s_1} dE(s)$$

$$\begin{aligned}
&= \frac{E_p(s_0)}{[\Delta t - s_0/c]} \int_{s_0}^{s_1} \exp[-\sigma(s - s_0)] \\
&= \frac{E_p(s_0)}{\sigma[\Delta t - s_0/c]} 1 - \exp[-\sigma(s_1 - s_0)].
\end{aligned} \tag{11}$$

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. As the photon travels from s_0 to s_1 , the energy it has is either lost to absorption, reaches census, or remains with the photon (in the form of sub-photons that haven't reached census yet). So the photon energy at s_1 is related to the photon energy at s_0 by

$$E_a(s_0, s_1) + E_c(s_0, s_1) + E_p(s_1) = E_p(s_0). \tag{12}$$

We know from Eq.(9) how the energy $dE(s)$ of a sub-photon is related to the energy E_p of the photon. We can use that to substitute for $E_p(s_1)$ in Eq.(12). This results in

$$E_a(s_0, s_1) = E_p(s_0)(1 - \exp[-\sigma(s_1 - s_0)]) \frac{\Delta t - s_1/c}{\Delta t - s_0/c} - E_c(s_0, s_1). \tag{13}$$

Although the results in this document show a problem in which the only source is thermal emission, the modified algorithm could be applied to other photon sources, such as face sources.

The advance of a source photon in the modified IMC algorithm consists of 4 steps.

Step 1 of is to calculate the following two quantities: the distance to the zone boundary $d_b(x_p, \Omega_p)$ and the distance to scatter $d_s = -\ln(r)/\sigma_s$. We take the minimum of these 2 distances: $d_p = \text{Min}(d_b, d_s)$.

Step 2 is to advance the photon a distance d_p . We change the photon's position $x_p \rightarrow x_p + \Omega_p d_p$, and we update the distance the photon has traveled in this time step $s_p \rightarrow s_p + d_p$. We calculate the amount of energy that reaches census and the amount that is absorbed via Eqs(11) and 13. These values are stored in the appropriate arrays, and the energy is removed from the photon.

Step 3 is to simulate the physical activity that was supposed to occur at the distance d_p . For example, if $d_p = d_s$, we would do a scatter, which would result in a change of Ω_p . If $d_p = d_b$, we move the photon to a new zone. Unlike standard IMC, we do not have a census event, because energy reaches census on every path.

Step 4 is to go back to step 1, unless the photon we are advancing has traveled a distance $s_p = c\Delta t$. As mentioned previously, this will also cause $E_p = 0$. Since we keep increasing s_p , the photon will eventually run out of energy, and the process will terminate.

There is one additional feature of the modified IMC algorithm that has to do with the fact that no photons reach census. We have calculated an amount of energy that reaches census in each zone, through the 4 step procedure outlined above. In the next time step, we need to represent this energy with photons. We can do this by randomly copying the source photons as we advance them. At the end of the time step, we give those copied photons energies that add up to the energy that reached census in the zone. These photons become census photons for the next time step, and are advanced like regular IMC photons. This is how the python code that implements the modified IMC algorithm

Now we will look at results for the test problems described in the previous section calculated by the modified IMC method. The first test is an infinite medium with initial values $T_m = T_r = 1.0$. The IMC results were depicted in Fig. 1. The modified IMC results are shown in Fig. 4

Fig. 4 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

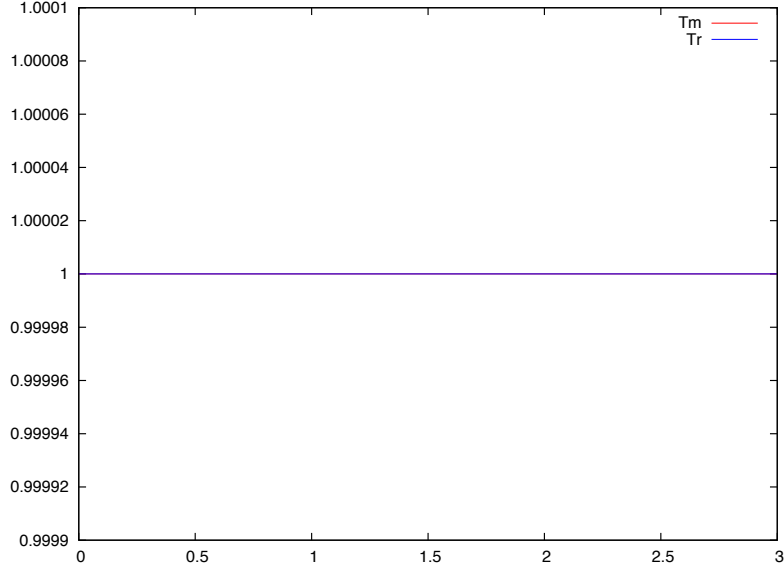


Figure 4: Matter and radiation temperature for infinite medium test problem using modified IMC with three different time steps

exactly the amount of energy calculated in Eq.(5) to census. In effect, the integrand in Eq.(6) 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 throughout the calculation.

Modified IMC results for the problems depicted in Figs. 2 and 3 are shown in Figs. 5 and 6 respectively. Both of these test problems begive out of equilibrium, and in both cases the modified IMC algorithm produces answers with no statistical noise.

The modified IMC algorithm completely eliminates the statistical noise in these infinite medium problems. This happens because the only source of statistical noise in these problems in the emission time. The position and direction of the photons are chosen using random numbers but do not effect the result. I don't expect such spectacular results in multi-zone problems. In those problems, there will be statistical noise from the position and direction, which will show up in how much energy gets deposited by the source photons that cross zone boundaries.

It is possible that the noise from photons the cross zone boundaries will completely swamp the reduction in noise we obtain by using the modified IMC algorithm. My hope is that we will see some reduction in noise in some circumstances. For example, problems with small Δt and large σ can have reletively few photons that cross zone boundaries. The modified IMC algorithm might show less noisy results on these problems.

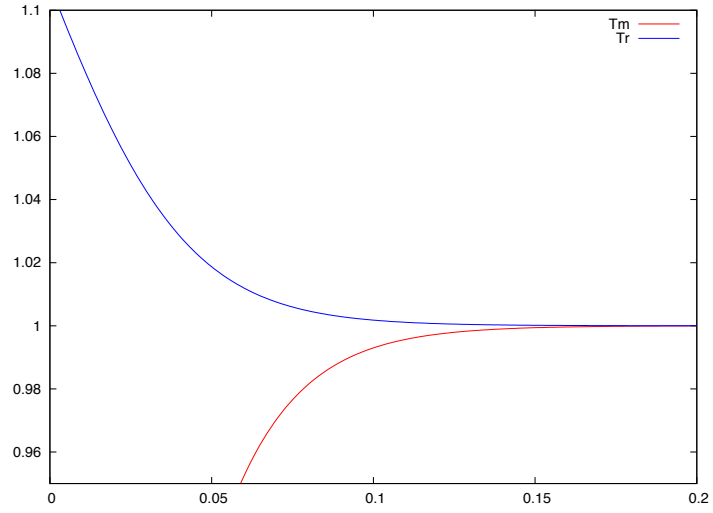


Figure 5: Matter and radiation temperature using modified IMC for infinite medium test problem with $T_r > T_m$ initially.

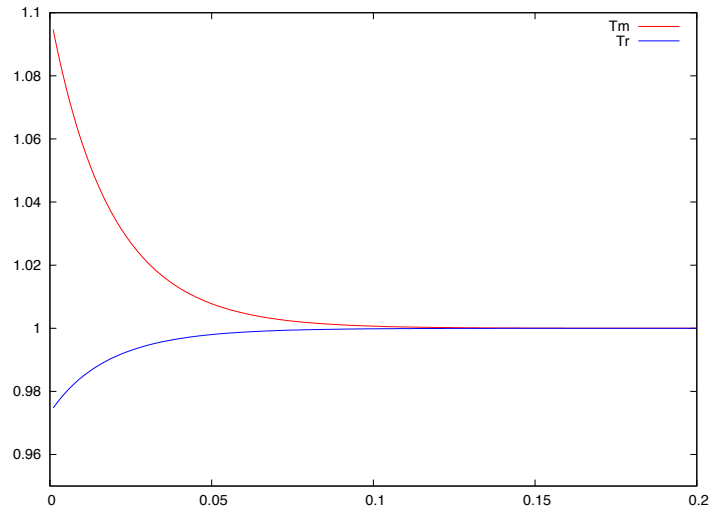


Figure 6: Matter and radiation temperature using modified IMC for infinite medium test problem with $T_m > T_r$ initially.

3. The student project

The IMC results shown in Figs. 1, 2 and 3 were generated by an IMC code written in c++. I have written a small python code implementing the modified IMC algorithm for an infinite medium problem. This is how the results shown in Figs. 4, 5 and 6 were generated. I want you to take the python code and, using that as a guide, put the modified IMC algorithm into the c++ code.

You will have to add a flag to the photon class in the c++ code that will mark the photon as either a census photon or a source photon. Census photons will be advanced by the same c++ code that they use now. The source photons will be treated by the new code you write. The new code will be very similar in structure to the already-existing IMC code. The python routines have almost the same names as the corresponding c++ functions (for example, `dBoundary` calculated the distance to the boundary, `advanceBoundary` takes the photon, calculated the absorption, and moves it to the boundary, etc.) So this task shouldn't be too daunting.

Once the modified IMC algorithm is coded into the IMC code, you can make sure that it reproduces the infinite medium test results of Figs. 4, 5 and 6. Then we'll try a multi-zone problem, like a 1D Marshak wave. An example of a Marshak wave problem is the one by Su and Olson, JQSRT 56 (1996), p. 337. IMC results for this test problem are shown in Fig. 7.

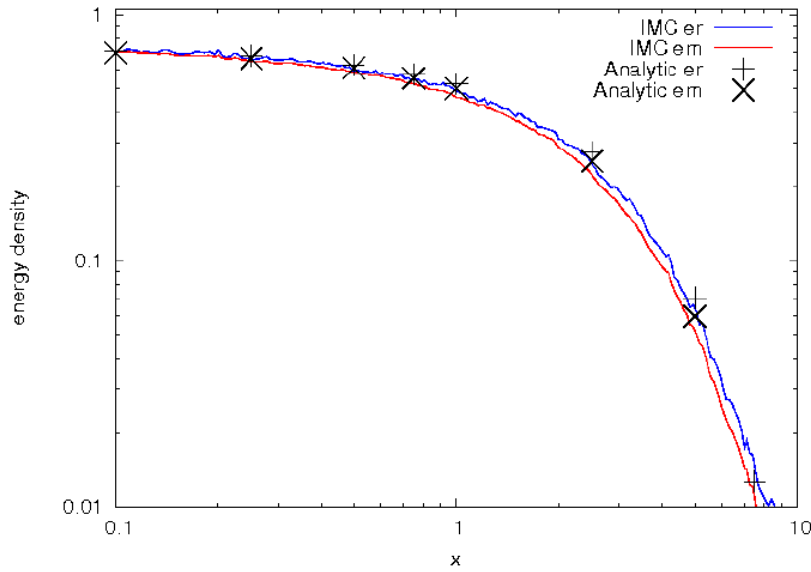


Figure 7: Matter and radiation energy for Su-Olson Marshak wave using IMC, compared to analytic answers

The Su-Olson Marshak wave has analytic answers, but only because it has a prescribed unphysical heat capacity and a fixed opacity. I think we want to test the modified algorithm on a

range of opacities, so we will use a different but similar problem. A more reasonable reasonable problem would be 10 or 20 zones spanning $x = [0, 1]$, with $T_m = T_r = 0.01$ and a $T = 1$ face source on it. We can change σ and Δt and see how the noise in the simulation varies.

After that, you make a talk, give it at Livermore. Then you can submit a write-up to an ANS conference and give the talk again. Possibly we will be able to take the results and this document and turn it into a paper for Journal of Computational Physics. I think the results in this document are good enough for an ANS talk, but I think we need to see that the modified IMC method works on a more realistic problem to make it worth a journal article.

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