IMPLICIT MONTE CARLO RADIATION TRANSPORT IN MULTI-PHYSICS SIMULATIONS

N. A. GENTILE
LAWRENCE LIVERMORE NATIONAL LABORATORY
L-38
5000 EAST AVENUE
LIVERMORE, CA 94550
gentile1@llnl.gov

ABSTRACT

This paper addresses the use of the Implicit Monte Carlo radiation transport technique in multi-physics simulations. We discuss how the features of this radiation transport algorithm contribute to and impact simulations involving hydrodynamics, laser ray tracing, and thermonuclear burn. We also discuss modifications of the algorithm needed for massively parallel computations, and address the issue of load balance.

Key Words: Monte Carlo radiation transport, multi-physics simulations

1. INTRODUCTION

The equations governing radiation transport coupled thermally to matter are [1]

\[
\frac{1}{c} \frac{\partial I}{\partial t} + \Omega \cdot \nabla I = - (\sigma_s + \sigma_a) I - \frac{1}{4\pi} c \sigma_a a T^4 b(\nu, T) + \int \sigma_s I \, d\nu \, d\Omega + S_i
\] (1)

\[
\frac{\partial \varepsilon}{\partial t} = \int \sigma_s I \, d\nu \, d\Omega - \sigma_a c T^4 + S_e
\] (2)

Here \( I(x, \Omega, \nu, t) \) is the radiation intensity, \( \sigma_a(T, \nu) \) is the absorption opacity, \( \sigma_s(T, \nu) \) is the scattering opacity, \( T(x, t) \) is the material temperature, \( b(\nu, T) \) is the normalized Planck function, \( \varepsilon(\rho, \nu) \) is the material energy density, and \( \rho \) is the material mass density. \( S_i \) and \( S_e \) are external radiation and matter sources, respectively.

These equations are linear in the radiation intensity. Because of this fact, a Monte Carlo algorithm may be used to solve the equation. However, the non-linearity in the matter temperature source term forces very short time steps to be used when this source term is differenced explicitly; that is, approximated using the value of the temperature at the beginning of the time step [2]. The Implicit Monte Carlo (IMC) radiation transport algorithm, developed by Fleck and Cummings, treats this source term semi-implicitly. This allows much larger time steps to be taken [3, 4].

The effect of the Fleck and Cummings semi-implicit linearization on Eqs. 1 and 2 is to reduce the absorption by a factor
\[ f_a = \frac{1}{1 + \beta c \sigma P \Delta t}, \]  
(3)

where the dimensionless quantity
\[ \beta = \frac{4 a T^3}{\rho c_v} \]  
(4)

and \( c_v \) is the heat capacity. A corresponding amount of scattering is added. That is, \( \sigma_a \) is replaced by \( f_a \sigma_a \) everywhere in Eqs. 1 and 2, and a new scattering term is added to Eq. 1:
\[
\frac{1}{4\pi} c \sigma_a b(\nu, T) \frac{\sigma_p}{\sigma_p} \int (1 - f_a) \sigma_a I d\nu d\Omega
\]
(5)

This added scattering has the same frequency distribution as thermal emission, and is referred to as effective scattering to distinguish it from the physical scattering described by the integral term in Eq. 1. The term \( f_a \) is often referred to as the “Fleck factor”.

With this modification, the method can be used to solve a wide array of radiation transport problems, including radiation hydrodynamics simulations, and simulations with other physics such as laser energy deposition, heat conduction, and thermonuclear reactions.

2. CHARACTERISTICS OF IMC WHICH HAVE A POSITIVE IMPACT ON MULTI-PHYSICS SIMULATIONS

IMC has several features that impact its usefulness for multi-physics simulations. First, we will discuss several positive features of IMC.

IMC, like Monte Carlo algorithms in general, is easily adapted to work in complicated geometries. This is because the most significant way that geometry comes into Monte Carlo algorithms is in tracking particles through the zones in the problem mesh. Most of the rest of the algorithm consists of zero-dimensional physics such as equation of state (EOS) and opacity calculations, and calculations that depend on the length of particle paths. Once this tracking problem is solved for a given mesh type (e.g., arbitrary polyhedra), Implicit Monte Carlo simulations are relatively straightforward, because the rest of the algorithm is unchanged.

Implicit Monte Carlo also simulates some physical processes with more fidelity than methods such as \( S_N \) and \( P_N \). For example, anisotropic scattering is handled easily, by changing the particle’s direction when scattering events occur [1]. Since IMC models scattering by deflecting the paths of particles in the simulation, it can represent the angular behavior of a scattering kernel with great fidelity. The angle of the scattered photon can be chosen from any given probability distribution. The same also applies to the frequency of the scattered photon, if the scattering kernel changes that quantity.
An example of a scattering kernel with a strong angular dependence is Thomson scattering [1]. If \( \mu \) is the cosine of the angle from the photon’s current direction, the probability distribution function for \( \mu \) is

\[
P(\mu) = \frac{3}{8} (1 + \mu^2).
\]  

(6)

This probability distribution function is strongly peaked in the directions \( \mu = 1 \) (the photon’s initial direction, and \( \mu = -1 \) (opposite to the photon’s initial direction).

Figure 1 shows the result of an IMC simulation of a beam of photons moving in the +z direction in a medium with negligible absorption opacity but a large Thomson scattering cross section. The dimensions of the beam and the material are 1 cm in the z direction and \( 10^{-6} \) cm in the x and y directions. This arrangement ensures that almost all of the photons will undergo one Thomson scatter from their initial direction of \( \mu = \Omega \cdot z = 1 \), but leave the medium before undergoing a second one. Tabulating the direction cosines of the photons leaving the mesh should then result in a distribution drawn from Eq. 6. Fig. 1 shows that this is the case.

This simulation used \( 5 \times 10^5 \) particles in the initial beam. The cosine of the angle of each scattered particle was tabulated and sorted into one of 20 equally sized bins in \( \mu \) in \([-1, 1]\). The number of binned particles divided by the total number is compared to the integral of Eq. 6 over the bin. The simulation took 3 minutes on 1 processor of an Opteron Linux cluster.

![Figure 1. Probability distribution of \( \mu \) for photons initially moving in +z direction that undergo one Thomson scatter.](image)
The IMC method can be modified to account for material motion in a relatively straightforward manner [5]. Thermal emission takes place in the fluid frame, and photons are Doppler-shifted into the lab frame for tracking. Given the photon’s lab frame direction, the lab frame absorption and scattering opacity can be calculated [1]. When scattering occurs, the photon can be Doppler-shifted into the rest frame of the fluid. The appropriate fluid frame scattering takes place, and the angle and frequency of the scattered photon is shifted back into the lab frame.

Let us examine the case where we measure the direction cosine $\mu$ from the direction of fluid motion ($\mu = 1$ points in the direction of fluid flow). The equation for the Doppler shift of the direction cosine $\mu$ in this case is

$$\mu_{\text{lab}} = \frac{\mu_{\text{fluid}} + \beta}{1 + \mu_{\text{fluid}} \beta},$$

where $\beta = v/c$, and $v$ is the fluid velocity. (This $\beta$ is not to be confused with the $\beta$ defined in Eq. 4.) As a consequence of Eq. 7, $\mu_{\text{lab}} - \mu_{\text{fluid}} \geq 0$, so Doppler shifting the fluid frame angle will produce a lab frame angle that is closer to 1. This means that scattering by a moving fluid is preferentially in the direction of fluid motion.

![Figure 2](image.png)

**Figure 2.** Probability distribution of $\mu$ for photons initially moving in the $+z$ direction that undergo one Thomson scatter in a material moving with $v = .9 c$ in the $+z$ ($\mu = 1$) direction.
Figure 2 shows the results of a simulation similar to the one previously described, but with the scattering material having a velocity of .9 c in the z direction. The scattering is now much more probable in the +z direction, since the fluid is moving in that direction. In this plot, the lab frame direction cosines were binned as described above.

The IMC simulation produces the correct distribution for a fluid moving with relativistic velocity. Deterministic methods are usually limited to first-order v/c corrections [5,6].

Multi-group calculations are also straightforward in Implicit Monte Carlo. Once the group structure is specified, the groups of thermally emitted photons can be drawn from a probability distribution function created by integrating the Planck function and the opacity over the group boundaries. Since the algorithm does not require solving a linear system for each group, the expense of IMC simulations grows more slowly with the number of groups than deterministic methods. This is in contrast to the behavior of deterministic simulations, for which run time usually scales approximately as the number of groups. For example, diffusion calculations usually have to solve at least one linear system for each group, so doubling the number of groups increases the run time by a factor of two.

This property of IMC simulations is illustrated in Figure 3. This figure depicts the results of an IMC simulation of a multi-group test problem with an analytic answer. A slab of brominated plastic (a material used in inertial confinement fusion experiments) has a density of .0916 g/cm$^3$ and an initial temperature of .03 keV. The slab is heated on one end with a temperature source at .3 keV. The heat capacity of the material is artificially taken to be $10^{50}$ ergs/g-keV, which forces the material temperature to remain constant. The absorption opacity is then constant, and the energy density of the photons in each group at a given point in space and time can be expressed in terms of exponential integrals. The derivation of the solution for a spherical medium is given in [7]. See [8] for the solution for slab geometry and details of this simulation.

This test problem was simulated using 50, 100, 200, and 500 groups. The run time for the simulations, which all used $3 \times 10^6$ photons and 16 processors on an Opteron Linux cluster, were as follows: 50 groups, 42.8 sec; 100 groups, 42.8 sec; 200 groups, 43.2 sec; 500 groups, 44.4 sec. The increase in run time is negligible, even though the number of groups increased by an order of magnitude. (These times are for the IMC photon advancement only; they exclude initial problem setup.)

Fig. 3 shows the energy density in each group for IMC simulations using 50, 100, and 200 groups, compared to the 200 group analytic answer. These values are for a point at a distance of 0.02 cm from the source, at a time $1.35 \times 10^{-12}$ sec from the beginning of the simulation. The groups were distributed logarithmically between $3.0 \times 10^{-3}$ keV and 30 keV.

The first peak in the figure, with a maximum at about .1 keV, is the thermal emission from the material at $T = 0.03$ keV. The second peak is caused by photons from the $T = .3$ keV source, which are absorbed in the low, opaque groups, but can stream through the high, less opaque groups. As the number of groups increases, the results for low energy groups become noisier, since there are fewer photons in each group. (This is why the 500 group results were not included in Fig. 3.)
3. CHARACTERISTICS OF IMC WITH A NEGATIVE IMPACT ON MULTI-PHYSICS SIMULATIONS

We will now discuss some characteristics of IMC that have a negative impact on multi-physics simulations.

The most vexing property of IMC calculations is noise, or statistical fluctuations. Monte Carlo methods exhibit statistical fluctuations in calculated quantities such as radiation energy density and temperature. This noise declines like $N^{-1/2}$, where $N$ is the number of particles used in the simulation [9]. Because the noise declines so slowly with the number of particles, it often takes many particles to produce an acceptably smooth answer. This can lead to very long run times for large simulations.

Besides providing an unpleasant appearance to simulations, the noise that IMC produces in quantities such as energy deposition can have a deleterious effect in radiation hydrodynamics simulations. For example, statistical fluctuations can seed hydrodynamic instabilities and perturb hydrodynamic flow in an unphysical way.

The statistical fluctuations also show up as poor resolution in parts of the simulation with low particle density. For example, since thermal emission is proportional to $\sigma_p T^4$ (where $\sigma_p$ is the

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Figure 3. IMC results for radiation energy density at a point in a heated slab of brominated plastic with a constant temperature and a multi-group opacity.
Planck mean opacity) most of the particles are radiated in hot opaque regions of the problem. Cold regions may not have enough photons to give an accurate solution. Since the frequency of thermally emitted photons is given by the Planck function, frequency groups with low energy content may have too few photons. (This is seen in the groups with lower energy in Fig. 3 above.)

The statistical fluctuations in the radiation temperature are apparent in Figure 4. This figure shows matter temperature from an IMC solution of a radiating shock, with a semi-analytic solution due to Lowrie and Edwards [10,11]. (Details of the test problem and solution will be provided in a later section.) This simulation has 1000 zones and was performed using $10^4$ photons. The noise in the radiation temperature compared to the semi-analytic answer is apparent in Fig. 4, particularly in the regions outside the shock, which are in thermal equilibrium. It is also apparent that the noise is larger ahead of the shock, where the lower matter temperature causes the simulation to employ fewer particles.

![Figure 4. Radiation temperature for Lowrie and Edwards [10,11] Mach 2 radiating shock from IMC simulation using $10^4$ photons compared to analytic answer.](image)

Noise in Monte Carlo simulations (more rigorously, the standard deviation of calculated quantities) scales as the square root of the number of particles. One way that noise can be reduced in some Monte Carlo simulations is by employing techniques that introduce correlations between particles, such as stratified sampling [9, 12]. Often in Monte Carlo calculations, some
initial quantity (such as particle time) is sampled randomly. Thus particles will cluster in some places and leave gaps in others. Stratified sampling attempts to “spread out” the particles to provide smoother coverage of the sampled space, while still using random numbers so that each part of the space has some probability of being sampled.

A simple problem illustrating the effects of stratified sampling is an infinite medium, with matter and radiation held at a fixed temperature. The medium has a constant heat capacity of $5.0 \times 10^{14} \text{erg/(g-keV)}$ and a constant opacity of $1.0 \text{cm}^{-1}$. Initially, the matter and radiation temperatures are set to $1.0 \text{keV}$, and the problem is advanced with time steps of $1.0 \times 10^{-10} \text{sec}$.

The radiation and matter temperatures should stay at the equilibrium value of precisely $1.0 \text{keV}$. However, they fluctuate around these values. (This is seen also in the equilibrium regions of Fig. 4.) The fluctuations occur because the emitted photons of the IMC algorithm have exactly the correct value of energy, $c\sigma T^4\Delta t$ per unit volume, but the times of emission are chosen randomly in $[t^n, t^{n+1}]$. For photon $i$, $t_i = t^n + r_i \Delta t$, where, $r_i$ is a random number unique to each photon. The amount of energy deposited by each photon depends on its initial time, so the deposition has some noise in it. This leads to values of matter and radiation temperature that fluctuate around the equilibrium value.

This noise can be reduced by sampling the emission times for the photons in a stratified manner. If $N$ photons are to be sampled in a give time step, photon $i$ has the initial time $t_i = t^n + (i + r) \Delta t/N$, where $r$ is a single random number used for all $N$ photons, and $i$ is a photon index between 0 and $N-1$. This distributes the photons initial time evenly across the time step – they are all separated by $\Delta t/N$ – with an offset that is different in each time step.

The effects of using stratified sampling for initial photon times are shown in Figure 5. Here we show the matter temperature for two IMC simulations of the infinite medium equilibrium problem described above, one of which employs stratified sampling for the initial photon times. Both simulations used 100 photons. The noise in the matter temperature is noticeably lower in the simulation that uses stratified sampling.

More interesting is the rate at which the noise declines with the number of particles. The noise is calculated as the standard deviation of the matter temperature in the last time step, using 30 simulations with different random number streams. This quantity is depicted in Figure 6. In this figure, the standard deviation of the temperature for the two different types of simulations are shown compared to best-fit power laws. The standard deviation of the matter temperature in the conventional IMC simulation declines as the number of photons to the $1/2$ power. For the IMC simulation employing stratified sampling of the thermally emitted photon initial times, however, the variance declines as $N^{-1}$, which is significantly faster than $N^{1/2}$. Stratified sampling of the thermally emitted photon’s initial time produces an answer for which the noise declines more rapidly with the number of photons.
Figure 5. Matter temperature vs. time for 2 IMC simulations of an infinite medium in equilibrium at 1 keV.

Figure 6. Matter temperature vs. time and standard deviation of final matter temperature for IMC simulations of infinite medium in equilibrium at 1 keV.
In the infinite medium test problem, the calculation of the photon’s initial time is the only significant event for which a random number is used, because position and direction are ignorable. In a multi-zone simulation, the initial position and direction of photons are also calculated using random numbers. In multi-group simulations, the same applies to photon initial frequencies. Stratification in more than one dimension is complex, because it is necessary to prevent correlations between different dimensions. (For example, we must ensure that the earliest photon emitted is not always chosen with the smallest x position in the zone.) Although the improvement in the noise is significant for this simple test problem, more research is required to determine if stratified sampling will improve the noise in simulations like that depicted in Fig. 4.

Another negative feature of IMC is the tendency of the temperature of material to overshoot, or increase too rapidly, when the energy sourced in during a time step is large compared to the mass times the heat capacity of a zone. IMC uses an estimate of the future matter temperature to calculate the thermal emission in the zone. This makes the method essentially equivalent to a semi-implicit discretization in time of the Eqs. 1 and 2 [3,4]. This semi-implicit discretization is more stable than purely explicit ones, but is much more prone to exhibit overshooting in simulations where the matter temperature or the radiation energy density are changing. This behavior is in contrast to that of a fully implicit discretization. When the source (or equivalently Δt) becomes large, fully implicit discretizations asymptote to an equilibrium value where matter temperature and radiation temperature are equal [13].

In order to reduce the amount of overshooting in IMC simulations, a heuristic limit on the magnitude of the change in matter temperature is used. It has been found useful to limit the change in matter temperature in any zone to be a factor of 10:

$$T^{n+1} - T^n \leq 10T^n.$$  (8)

If the temperature change in a zone exceeds this limit, an amount of energy necessary to reduce the temperature is removed from the zone. This energy is added back into the zone in the next time step. Since the temperature of the zone has increased, the “Fleck factor” will be smaller in the next time step, and the absorption opacity is likely to be smaller also. This will cause the effective absorption to be smaller on the next time step, and so the energy that is added back in will cause a smaller increase in the temperature than it would have in the previous time step.

This limit is deliberately coarse because small, cold zones in simulations may absorb enough energy to increase their temperature significantly. It is usually preferable to let these cold zones heat up rapidly, rather than trying to resolve their temperature change more accurately by cutting the time step to a very small value.

An example of the overshooting that can occur with IMC is provided by the following test problem. We take a slab of material 2 cm long, divided into 200 zones with a constant width of .01 cm. The material has a constant $c_v = 10^{16}$ erg cm$^{-3}$ keV and a constant absorption opacity of $\sigma = 100$ cm$^{-1}$. The initial temperature is .01 keV. The slab is heated by a temperature source of 1 keV at x = 0. The simulation employs a constant time step of $10^{-11}$ sec. We examine the temperature in the first zone of the simulation.
As the material heats up, it should never exceed the source temperature of 1 keV. As shown in Figure 7, however, an IMC simulation produces a temperature larger than 7.8 keV is obtained in the first zone at the end of the first time step. The temperature declines slowly from there until it finally approaches the equilibrium value of 1 keV after nine time steps. An IMC simulation that does employ the limiting procedure reaches a maximum temperature of 1.2 keV, and declines to the equilibrium value on the fifth time step. These simulations are compared to an IMC simulation that used a smaller time step, $10^{-12}$ sec. This simulation does not exhibit overshooting. For this test problem, the temperature limit procedure allows us to use a time step 10 times larger while holding the overshoot in the temperature to a tolerable level.

**Figure 7.** Temperature of first zone in an IMC simulation of a heated slab, with and without temperature limiting.

### 4. IMC SIMULATIONS OF RADIATING SHOCKS

Lowrie and Edwards [10, 11] have constructed a radiating shock test problem, with ideal gas EOS and analytic opacity, which has a semi-analytic answer. The effects of radiative transfer are treated by solving the nonequilibrium diffusion equation, which is a good approximation to transport when the opacity is large. The solution consists of a radiating shock traveling in a self-
similar manner. Given the correct initial conditions, a radiation-hydrodynamics simulation should preserve the shape of the solution, shifting it in time by the (constant) shock speed multiplied by the elapsed problem time.

This problem was simulated using IMC and one-dimensional ALE hydrodynamics in the ICF code Kull [14, 15]. The mesh used 1000 zones, which were of equal size and spanned \( x = [0.01 \text{ cm}, 0.11 \text{ cm}] \) at \( t = 0 \). The IMC simulation used \( 1.0 \times 10^6 \) photons. The material is an ideal gas with \( \gamma = 5/3 \) and a heat capacity of \( 2.22 \times 10^{15} \text{erg/(g-keV)} \). The unperturbed density is \( 1.0 \text{ g/cm}^3 \), and the unperturbed matter and radiation temperatures are both 0.122 keV. The opacity has a constant value 577.3 cm\(^{-1}\). The shock velocity is \(-3.46 \times 10^7 \text{ cm/sec}\), which is Mach 2. The shock results in a final density of 2.29 g/cm\(^3\), a final velocity of \(-1.95 \times 10^7 \text{ cm/s}\), and final matter and radiation temperatures of 252.5 keV.

The analytic solution was used for the initial conditions of the simulation, with the initial shock position at \( x = 0.09 \text{ cm} \). The boundaries of the problem both had a fixed velocity and incoming radiation flux, derived from the initial velocity and radiation temperature respectively. The simulation was run to a time of \( 1.73 \times 10^{-9} \text{ sec} \), by which time the shock moved to \( x = 0.03 \text{ cm} \), through about 700 zones. The simulation took 1.4 hours on 80 processors of an Opteron Linux cluster.

Figures 8-11 show the mass density, velocity, matter temperature and radiation temperature respectively for the Mach 2 shock. Both the initial values and the final analytic and calculated values are shown. The IMC results for all the quantities look very similar to the analytic solution in both shape and location, which shows that the IMC radiation hydrodynamics solution accurately reproduces the analytic answer.

Some differences between the radiating shock and a non-radiating shock are apparent in Figs. 8-11. Radiation from the heated matter behind the shock heats matter ahead of the shock. So the temperature of the matter ahead of the shock starts to increase before the shock reaches it, in contrast to the familiar hydro-only planar shock. The shocked matter is not in equilibrium; it has a higher matter temperature than radiation temperature for some distance behind the shock. As the shocked matter cools, it continues to increase in density, so the density continues to rise even after the shock has passed, and the velocity continues to decline. Matter temperature is discontinuous in the shock, but radiation temperature is continuous.

Statistical fluctuations in the radiation temperature are visible in Fig. 11. The radiation temperature shows more statistical fluctuations than the matter temperature. This is because the radiation temperature for a time step is calculated from the energy of photons that passed through a zone during that time step, while the matter temperature is calculated from energy deposition and emission events that occurred in all previous time steps. More photon events contribute to the calculated value of matter energy and temperature, thus making them noisy.

Lowrie and Edwards have also provided a semi-analytic solution for a radiating shock with a variable opacity [11]. For the particular simulation presented here, the shock is Mach 2, and the EOS and post and pre-shock values of density, temperature, and velocity are the same as for the constant opacity shock described above. The opacity has the value
Figure 8. Density for Mach 2 radiating shock compared to the analytic answer.

Figure 9. Velocity for Mach 2 radiating shock compared to the analytic answer.
Figure 10. Matter temperature for Mach 2 radiating shock compared to the analytic answer.

Figure 11. Radiation temperature for Mach 2 radiating shock compared to the analytic answer.
\[ \sigma = \sigma_0 \rho T^{-3.5}, \]

where \( \sigma_0 = 0.362 \text{ cm}^2/(\text{g } \text{keV}^{-3.5}) \). That is, \( \sigma \) is in \text{cm}^{-1} if \( \rho \) is in \( \text{g cm}^{-3} \) and \( T \) is in keV. The unperturbed opacity has the same value as the constant opacity of the previously described Mach 2 shock, 577.3 \text{ cm}^{-1}. The final opacity is lower, with a value of 102.1 \text{ cm}^{-1}. The final mean free path, although smaller than the unperturbed value, is still small compared to the scale of the shock. Because of this, we can expect that the diffusion approximation used to obtain the semi-analytic answer will be accurate enough to approximate transport. IMC simulations of this test problem confirm this. This simulation, like the previously described one, was run to a time of \( 1.73 \times 10^{-9} \text{ sec} \), and the shock moved to the same position, \( x = 0.03 \text{ cm} \), through about 700 zones. The simulation took 2.5 hours on 80 processors of an Opteron Linux cluster.

Figures 12-15 show the density, velocity, matter temperature, and radiation temperature respectively for the variable opacity shock problem. Both the initial values and the final analytic and calculated values are shown. As above, the IMC simulations used \( 10^6 \) photons.

The features of the solution of the variable opacity radiating shock are similar to those of the constant opacity solution. This is not surprising, because the change in opacity affects the rate at which the matter and energy reach equilibrium, but not the overall energetics of the shock. The decrease in the opacity as the temperature rises allows the radiation from the shocked matter to penetrate further into the pre-shocked material. The lower opacity of the post-shocked material means that it takes longer for the matter temperature to decline to the radiation temperature. The pre- and post-shock effects of radiation take place over a greater distance than is the case for the constant opacity radiating shock. (Note that the distance scales of Figs. 12-15 are larger than the scales of Figs. 8-11 to reflect this.)

The agreement between the IMC simulations and the semi-analytic answer is not quite as good as that obtained with the constant opacity shock problem, as seen in Figs. 8-11. Compared to the semi-analytic answer the simulation produces a radiation temperature that is lower in front of the shock and higher behind it. The matter temperature from the simulation is lower in front of the shock, but in good agreement behind it. There are also differences in the density and velocity around the shock. The shock location, however, is reproduced very accurately in the simulation, even though a large fraction of the mesh has been traversed by the shock.

Whether these differences are the result of transport effects in the IMC simulation that are not accounted for in the diffusion approximation, or are vagaries of the numerical simulation awaits further investigation. Comparison to flux-limited diffusion and \( S_N \) simulations should help shed some light on these issues.
Figure 12. Density for variable opacity radiating shock compared to the analytic answer.

Figure 13. Velocity for variable opacity radiating shock compared to the analytic answer.
Figure 14. Matter temperature for variable opacity radiating shock vs. analytic answer.

Figure 15. Radiation temperature for variable opacity radiating shock vs. analytic answer.
5. IMC SIMULATIONS OF ABLATIVELY DRIVEN RAYLEIGH-TAYLOR INSTABILITY

If a dense fluid is accelerated into a less dense fluid, the interface between the fluids suffers from an instability called the Rayleigh-Taylor instability [16]. If the interface between the fluids was initially planar, it becomes more convoluted with time as fingers of the more dense fluid penetrate into the less dense fluid. While the displacements of the fluids remain small, the development of the interface can be approximated by linearized hydrodynamics equations. In this regime, an analytic solution for the development of the interface can be obtained [17]. As the perturbation grows, the non-linear development can be investigated by hydrodynamics simulations.

Since many inertial confinement fusion (ICF) experiments involve a heavy material being accelerated into a lighter one, Rayleigh-Taylor instability simulations are of interest in ICF applications [18]. In an ICF simulation, the material motion is usually caused by illumination from a laser. Heating from the laser causes part of the material to ablate, which imparts a force to the rest of the material, accelerating it. If this accelerated material impacts a less dense material, the interface will manifest the Rayleigh-Taylor instability.

A simulation that tests the ability of codes to model an ablatively driven Rayleigh-Taylor instability is easy to construct. The simulation consists of a region of a hydrogen-helium mixture, the light fluid, which has a $\frac{1}{2}$ wave sinusoidal interface with brominated plastic, the heavy fluid. The interface runs in the x direction, in which both fluids span $4.0 \times 10^{-3}$ cm. The H-He mixture has an extent of .1 cm in z direction, and the brominated plastic spans $4.0 \times 10^{-3}$ cm. (The y direction is ignorable.) The initial density of the H-He mixture is $8.33 \times 10^{-4}$ g/cm$^3$. The initial density of the brominated plastic is 1.05 g/cm$^3$. The initial temperature of both materials is $1.72 \times 10^{-4}$ keV (2000 K). One end of the H-He mixture is illuminated by a time dependent radiation source, which mocks up the effects of laser illumination.

The simulation was run on two different meshes in the ICF code Kull. One mesh had 10 zones in the gas and 30 in the plastic along z, and 30 zones in x. This mesh had 1200 total zones. The other one doubled the resolution in both z and x, for a total of 4800 zones. Both meshes had one zone in the ignorable y direction, and both had fine zoning around the interface in the brominated plastic.

Flux-limited diffusion (FLD) and IMC were both used for simulations on both meshes. The IMC simulation on the 1200 zone mesh used $8.0 \times 10^5$ photons, and the simulation on the 4800 zone mesh used $3.2 \times 10^5$ photons. Run time for the IMC runs were 1.85 hours on the 1200 zone mesh, and 7.72 hours on the 4800 zone mesh.

The figure of merit for these simulations is obtained by integrating the density along the z direction from one end of the mesh to the other. For a given time, this results in a function of x only, called the “areal density”. The areal density is then Fourier transformed. The magnitude of the coefficient corresponding to the wavelength of the original perturbation is calculated. This component is the figure of merit.
The reason that this quantity is significant is that it can be measured in an experiment, by passing a beam of x-rays along the z-axis. The absorption of the x-rays probes the density in the z direction, effectively integrating it. The resulting intensity of the x-rays, as a function of x, can be Fourier transformed to obtain a measurement of the figure of merit calculated from the areal density.

Figure 16 shows the density and material boundary of the IMC simulation on the more refined mesh at 3 different times. The first segment of Fig. 16 shows the part of the mesh which contains the interface between the two materials at $t = 0$. The fine zoning between the materials can be seen. The second segment shows the same part of the mesh at $t = 1.1 \times 10^{-9}$ sec. The ablation of the brominated plastic into the H-He mixture can be seen by the location of the pink line marking the material interface. The ablation of the outer part of the plastic is compressing the inner part to a greater density. The third segment shows the whole mesh at $t = 3.3 \times 10^{-8}$ sec. The compressed part of the plastic in the upper part of the plot has started to assume a complicated shape. Soon after this, the simulation ended as the mesh motion caused the formation of a negative volume zone.

The figure of merit for all the simulations, as a function of time, are shown in Figure 17. At early times, all simulations produce similar results. Only the FLD simulation on the less-resolved mesh completed. The meshes tangled in the other three simulations. In this simulation, the
amplitude of the perturbation rises, and then decreases. This is the desired result from the perspective of ICF experiments, because decreasing the effect of the instability would lead to more compression of the ablated material [17,18]. However, the other simulations tangle before completing, so it is not clear that this result is physical. The other simulations all show a larger amplitude for the instability. It is possible that the IMC simulations are more likely to tangle because the discrete impulses provided by the individual IMC photons seed the instability. To determine if this is the case, further simulations with more photons are necessary. Experimenting with the parameters of the ALE hydrodynamics could also produce more robust simulations of this test problem.

Figure 17. Figure of merit for simulations of an ablatively driven Rayleigh-Taylor experiment.

6. IMC SIMULATIONS OF AN ICF PROBLEM

The ICF calculation depicted in Figure 18 used IMC in conjunction with ALE hydrodynamics, laser energy deposition, and electron heat conduction in the ICF code Hydra [19]. This simulation used $4.8 \times 10^6$ IMC particles. Laser energy is deposited on the inner surface of the cylinder (light blue in the material boundary plot) containing the ICF target (the red sphere in the material boundary plot in Fig. 18.) Radiation from the hot regions created by the lasers fills the
cylinder, as depicted in the radiation temperature plot. Radiation pressure compresses the ICF target, leading to conditions that can cause fusion.

This simulation demonstrates both the strengths and weaknesses of IMC.

The region has a complex three-dimensional geometry that changes during the simulation because of material motion. As noted above, IMC is easily adapted to challenging geometries. This simulation has a cylinder of opaque material containing a large region with low opacity. Very little of the opaque cylinder become hot; most of the thermal energy is in the low opacity material. IMC runs relatively rapidly in simulations that do not contain large amounts of hot opaque material.

A weakness of IMC, the statistical fluctuations, is also demonstrated in this simulation. Because the ICF target is compressed by ablation of heated, and hence less dense, material from its surface, it is subject to hydrodynamic instabilities. The noise in the IMC energy deposition can seed this instability. This noise can be suppressed by a numerical averaging procedure, which is performed on the energy deposition in the zones on the surface of the ICF target.

Figure 18. Material boundaries and radiation temperature for Hydra simulation of three-dimensional ICF experiment.

7. PARALLEL IMC SIMULATIONS

Implicit Monte Carlo simulations can be run in parallel in several different ways. If the entire problem domain (i.e., the mesh and other variables) can be fit on one processor, then the problem can be run faster by simulating multiple copies on several processors. In this parallelization
scenario, each processor completes computations involving a fraction of the particles. Quantities aggregated over all particles, such as energy deposition, are then summed over all processors. This approach is referred to as mesh replication.

In most IMC simulations, the computations that advance the particles from the beginning to the end of the time step take up most of the time of the simulation. The “overhead” – operations like calculating opacities, EOS quantities, and mesh quantities needed for tracking – are usually a small fraction of the simulation time. When this condition holds, the run time of a mesh replicated IMC simulation falls in proportion to the number of processors. When a simulation’s run time is proportional in this way, it is said to be “embarrassingly parallel.” The embarrassingly parallel nature of an IMC simulation is illustrated in Figure 19.

Fig. 19 shows run time versus processor number for IMC simulations of the Su-Olson test problem, a one-dimensional radiation-only test problem with a semi-analytic answer [20]. A volume radiation source heats part of a slab of material for a given time. Radiation from the source and thermally emitted radiation flow into the unheated regions of the slab. The EOS of the material is selected to make the coupled transport and matter energy equations linear. This permits their solution to be expressed as integrals that may be solved numerically. (See [20] for details and tables of the solutions for both transport and diffusion.)

Figure 19. Run time vs. processor number for mesh replicated simulations of the Su-Olson test problem
This simulation used $10^6$ photons and a mesh with 200 zones. Because the mesh is small, a copy can be fit on every processor. The ideal scaling of the run time is $1/N$, where $N$ is the number of processors. For this test, we achieve almost ideal scaling until more than 64 processors are used.

When the problem is too large to fit on one processor, it must be broken up into several domains. This approach is referred to as domain decomposition. The IMC algorithm can be employed in this domain decomposed mode, once certain changes involving trading particles among processors are made [21]. Because particles can move to domain boundaries at any time during the simulation, an unknown number of messages, of unknown size, must be sent at various times during each time step of the simulation. Determining when the time step is complete can also be difficult, both because particles may be in transit, and because the number of particles in the simulation may change. This can occur if particles can be split, for example [22].

Because there are more particles in hotter, more opaque zones, the number of particles on each domain may vary considerably. Thus a small region of the problem may consume a large fraction of the computational resources. This situation is referred to as load imbalance. A simulation suffering from load imbalance may not run much faster than one run on a smaller number of processors. This will be the case when the domain decomposition does not spread out the most computationally expensive regions over many processors.

Figure 20 compares mesh replication and domain decomposition for the Su-Olson problem described above. This figure plots run time for both mesh replicated and domain decomposed simulations with the same number of processors. This problem has a source in one region, which in these simulations is the left quarter of the zones. More photons are present in this region than in the others. Since domain decomposition devotes processors to regions of the mesh that contain fewer photons than the source region, the run time falls much less quickly than the $1/N$ behavior exhibited in the mesh replicated case.

Load imbalance may be addressed by combining domain decomposition and mesh replication. We refer to this as domain replication. After the problem is domain decomposed, multiple copies of the most expensive domains are replicated. This replication is done so that each processor has an approximately equal amount of work, which leads to better efficiency. The algorithm described in [22] can be adapted for this case. Two changes are necessary.

First, it is possible for particles that cross a domain boundary to have several possible destinations, since each domain may have more than one copy. This is dealt with by “round-robinning” the particles into a set of buffers, one for each possible destination. Each particle buffer then behaves as described in [22].

Second, it is necessary to do sums of quantities such as energy deposition over the subset of the processors that are simulating a copy of the same domain. This requires the construction of a separate MPI communicator for each domain.
Figure 20. Run time vs. processor number for mesh replicated and domain decomposed simulations of the Su-Olson test problem

Figure 21. Run time vs. processor number for mesh replicated and domain replicated simulations of the Su-Olson test problem
Domain replication is illustrated in Fig 21. This figure depicts the run time of the Su-Olson test problem with various numbers of processors with various numbers of copies of each domain. The red line describes 2 domain simulations with one copy of domain 1, which does not contain the source. The pink line describes simulations with 2 copies of domain 1. The black line describes pure domain decomposed simulation (one processor for each domain). The mesh replicated simulations (blue line) are still the fastest, but if one were forced to use domain decomposition, choosing the processor distribution wisely can lead to run times that are not too far from optimal. For example, given four processors, three copies of domain 0 (the source domain) and 1 copy of domain 1 is much faster than 2 copies of each domain, or a single copy of 4 domains. Given 16 processors, a 14-2 apportionment is better than a 15-1 apportionment, and both are much better than a domain decomposed simulation with 16 domains.

The utility of domain replicated simulations in a radiation hydrodynamics simulation is illustrated by the problem shown in Figure 22. This simulation consists of a slab consisting of Si O$_2$, which has a relatively small opacity, and plastic, which has a larger opacity. The surface of the Si O$_2$ at $x = 10$ cm is heated with a time-dependent temperature source, which causes radiation to stream through and impinge upon the more opaque plastic at $x = 5$ cm. The plastic heats up and ablates, launching shocks in both directions.

![Figure 22. Depiction of a radiation hydrodynamics test problem. Plastic (red) spans $x = [0, 5 \text{ cm}]$ and Si O$_2$ (green) spans $x = [5 \text{ cm}, 10 \text{ cm}]$. A heat source is imposed at $x = 10$ cm.](image)

This problem was simulated on a very large mesh to test the IMC domain replication algorithm. Three different simulations were done on a mesh with about 570,000 zones. One employed 512 domains with one copy each. One employed 128 larger domains, with 4 copies each. The last employed the same 128 domains as the second, but with various numbers of copies of each domain. The number of copies of the domains in the last simulation was determined by looking at the number of IMC photons simulated in each domain throughout the second simulation. The number of copies varied between 1 and 12. We refer to the situation where a simulation has unequal numbers of copies of the domains as uneven domain replication.
The run time for the 512 domain simulation was 18.4 hours. The run time for the 128 domain, 4 copy simulation was 11.9 hours. The run time for the unevenly domain replicated simulation was 5.55 hours. The advantage of uneven domain replication is significant. All simulations used 512 processors of an Opteron Linux cluster.

Other physics packages will have a different strategy for optimizing computer resources. For example, most hydrodynamics algorithms expend about the same amount of computational effort in each zone. The optimum decomposition for a hydrodynamics package will be to decompose the problem into a large number of domains with an equal number of zones. This can conflict with the optimum strategy for IMC, which would involve replicating expensive domains.

In the radiation hydrodynamics simulation described above, the hydrodynamics algorithm was run using the same domain decomposition as the IMC. The hydrodynamics calculations are done on every domain. This means that, for domain replicated simulations, hydrodynamics work was duplicated for domains that had more than one copy. This strategy was employed for 2 reasons. First, it is simple to code, and second, it eliminates any need to communicate the results of the hydrodynamics calculations between processors. But this strategy has the drawback that the simulation is sub-optimal from the point of view of hydrodynamics.

The amount of sub-optimality can be estimated by looking at the fraction of time spent in IMC compared to the rest of the simulation. (Most of the remainder is hydrodynamics with a small fraction being serial overhead like EOS and opacity simulations.) The 512 domain decomposed simulation spent 94% of its time in IMC. The 128 domain, 4 copy simulation spent 75% of its time in IMC. The uneven domain replication simulation spent 55% of its time in IMC. To obtain significant decreases in run time for this simulation by increasing the number of processors, we would need to make smaller domains rather than more copies of existing ones. This is true because the expense of the IMC no longer dominates the run time.

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