Improved Convergence Rates In Implicit Monte Carlo Simulations Through Stratified Sampling

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INTRODUCTION

The Implicit Monte Carlo (IMC) method solves Thermal Radiative Transport problems by simulating the history of individual photons. These simulated photons have properties set by sampling from distribution functions in space, angle, frequency and time. Because the sampling process is random there is no guarantee that all portions of phase space will be represented. Stratified sampling overcomes this deficiency by subdividing all of phase space into bins such that the total number of bins represent the number of simulated photons. We show that this method improves the convergence rate and figure of merit (FOM) for various gray problems.

DESCRIPTION OF ACTUAL WORK

IMC Equations

The IMC as derived by Fleck and Cummings [1] method effectively linearizes the TRT equations. The gray IMC equations for the radiative and material energy balance are:

$$\frac{1}{c}\frac{\partial I(\mathbf{x},\Omega,t)}{\partial t} + \Omega\cdot\nabla I(\mathbf{x},\Omega,t) + \sigma_{a,p}I(\mathbf{x},\Omega,t)$$
$$= \frac{1}{4\pi}\sigma_{a,p}fcaT^4(\mathbf{x},t) + \frac{1}{4\pi}\sigma_{a,p}(1-f)\int_{4\pi} I(\mathbf{x},\Omega',t)d\Omega' \quad (1)$$

$$\frac{\partial U_m}{\partial t} = \int_{4\pi}\sigma f I(\mathbf{x},\Omega,t)d\Omega + \sigma_{a,p}facT_m^4(\mathbf{x},t) \quad (2)$$

The intensity is a function of six variables. When a photon is created it is given some representative energy-weight and then its properties are sampled from probability density functions (PDFs). Within a discrete cell, photons are assumed to be emitted uniformly in angle (that is, uniform in the cosine of the polar angle and uniform in the azimuthal angle), space and time. If the problem is not gray the frequency is sampled from a Planckian at the temperature of the discrete cell. The PDFs differ if photons are being emitted from a non-uniform source or if some form of tilting is used.

Stratified Sampling

The impetus behind stratified sampling is to represent as much phase space as possible with a finite number of samples. (!! Include Author of sampling paper!!) showed that if stratified sampling is used for Monte Carlo integration the convergence rate of the solution improves to $O(N^{-(1+2/D)})$ where D is the number of dimensions that have been stratified. To employ stratified sampling the PDFs for space, angle and time must be divided into some number of bins: x_b, y_b, z_b, μ_b, ϕ_b, t_b. Phase space is thus represented as a cube where the total number of bins is

$$N_{bins} = x_b y_b z_b \mu_b \phi_b t_b. \quad (3)$$

Within each of these bins, the dimension is sampled uniformly, e.g. a photon in the 8$^{\text{th}}$ x bin would have some random position between the 8$^{\text{th}}$ and 9$^{\text{th}}$ bin. In an ideal case the total number of bins would be equal to the number of simulated photons, $N_p = N_{bins}$ and each dimension of phase space would be divided into an equal number of bins. In that case the number of bins for a given dimension would be:

$$x_b = y_b = z_b = \mu_b = \phi_b = t_b = N_{photons}^{\frac{1}{6}}. \quad (4)$$

In practice, the number of photons in a given discrete cell of the problem does not have an integer sixth root. It would be possible to make more photons in a cell with less energy-weight to satisfy Eq. (4) but having photons with differing energy weights from cell to cell would likely negatively offset the benefit of stratified sampling. Instead, we take the floor of the sixth root and then increase the number of bins in a given dimensions by a factor of two until this would cause $N_{bins} > N_{photons}$. When sampling we then use all bins in our now rectangular six dimensional parameter space and then randomly reuse bins until we have sampled all photons.

RESULTS AND ANALYSIS

Stratified sampling was implemented in the FINMCOOL code developed by Nuclear Engineering students at Texas A&M University. The results in this paper compare absolute error and simulation run time and total figure of merit to evaluate the efficacy of the algorithm. The figure of merit could be better than the results shown here as the authors make no claim that the implementation of stratified sampling in the code is ideal.

0D Equilibrium

For a truly zero dimensional problem grey problem there is no need to stratify any of the variables except time. Because the solution is only a function of one variable we can stratify that variable exactly ($t_b = N_{photons}$). Here a 0D problem at 1.0 keV was run with a 1 nanosecond time step. Figure (1) shows

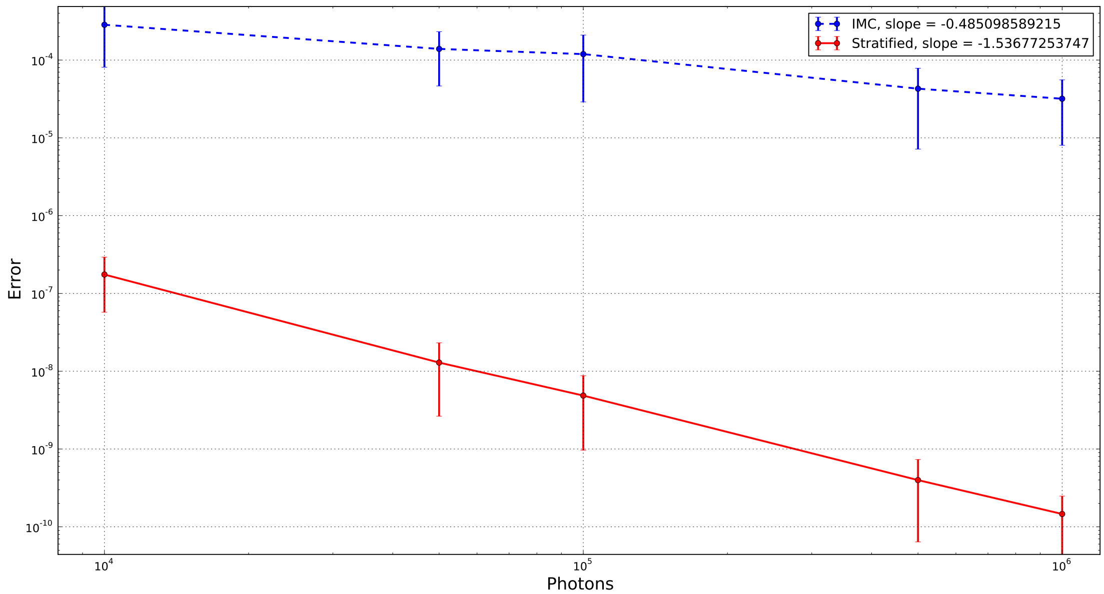

Fig. 1. Error vs. number of photons for a 0D problem at equilibrium after one timestep

Method	Photons	Run Time (s)	Error	FOM
Stratified IMC	5e7	108.53	0.0069	1.335
IMC	5e7	106.16	0.01337	0.704

that we obtain roughly the ideal improvement in convergence rate as shown in Eq. (!!!!).

Infinite Medium Equilibrium

A simple infinite medium problem at equilibrium was run to test the algorithm with all six dimensions stratified. In this problem the initial and final temperature is 1.0 keV. A 1.0 cm cube was used with five spatial zones in each dimension. The opacity is 1.0 cm^{-1} and the heat capacity is 1.0e7 $\frac{\text{jk}}{\text{g keV}}$. The heat capacity is set unphysically high to eliminate effective scattering so the benefits of angular stratification can be tested. Fig. (2) shows the results after one 0.01 sh time step. A linear fit gives a slope of about -0.58 for the IMC with stratified sampling. The ideal -0.66 convergence rate predicted in Eq. (!!) is for an infinite number of particles. The convergence rate does seem to improve–the slope between 1e7 photons and 5e7 photons is about -0.68. Fig. (3) shows that the implementing stratified sampling does not significantly impact run time. The Figure of Merit for 5e7 photons is shown in the following table:

A second equilibrium problem was run with more realistic parameters. The opacity was set to 1.0 cm^{-1}, the heat capacity to 0.1 $\frac{\text{jk}}{\text{g keV}}$ and the same time step size was used. This problem has a Fleck factor of about 0.79, so the scattering ratio is about 20%. After one time step the error for varying number of photons is shown in Fig. 4. Fig 4 shows that even with some degree of scattering convergence rates improve but scattering does decrease the rate of convergence with stratified sampling.

CONCLUSIONS

Stratified sampling can be used to improve the convergence rate and Figure of Merit for TRT problems. The algorithm is not expensive to implement and when the problem is optically thin FOM can be improved by a factor of two. The degree of scattering in the problem will tend to make stratification in angle less important–angle is resampled uniformly after a scattering interaction, thus the solution will behave as if the angular variables were not stratified.

Stratified sampling could easily be extended to frequency dependent problems. It also may be possible to obtain better results on problems with high scattering ratios by turning off stratification in angle at a certain point to create more bins in space and time.

REFERENCES

1. J. A. FLECK and J. D. CUMMINGS, “An Implicit Monte Carlo scheme for calculating time and frequency dependent nonlinear radiation transport,” *J. Comp. Phys.*, **8**, 313–342 (1971).

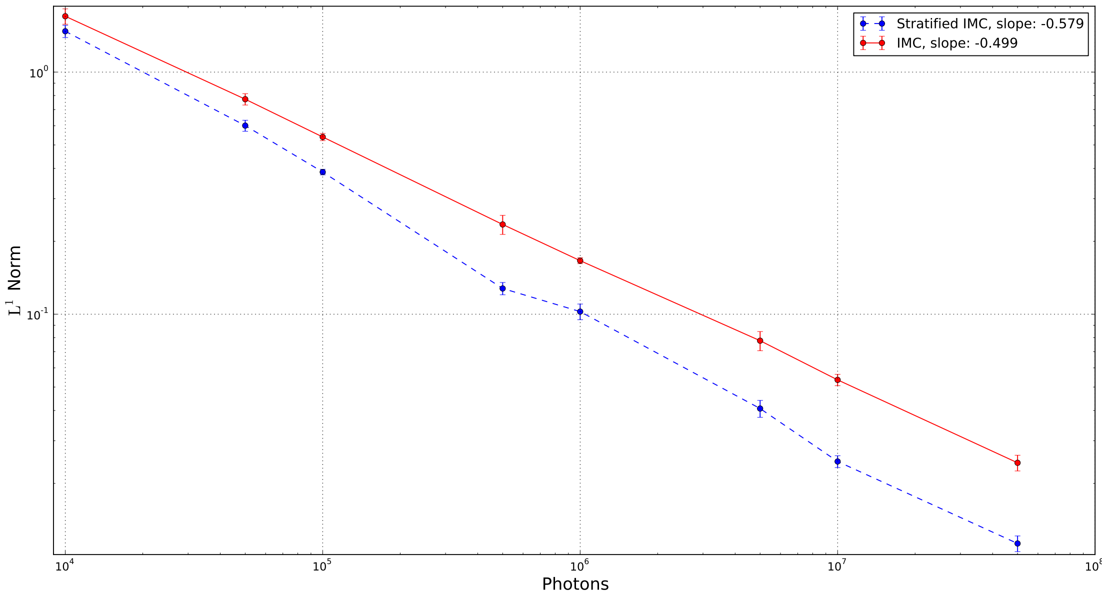

Fig. 2. Error vs. number of photons for a 0D problem at equilibrium after one timestep

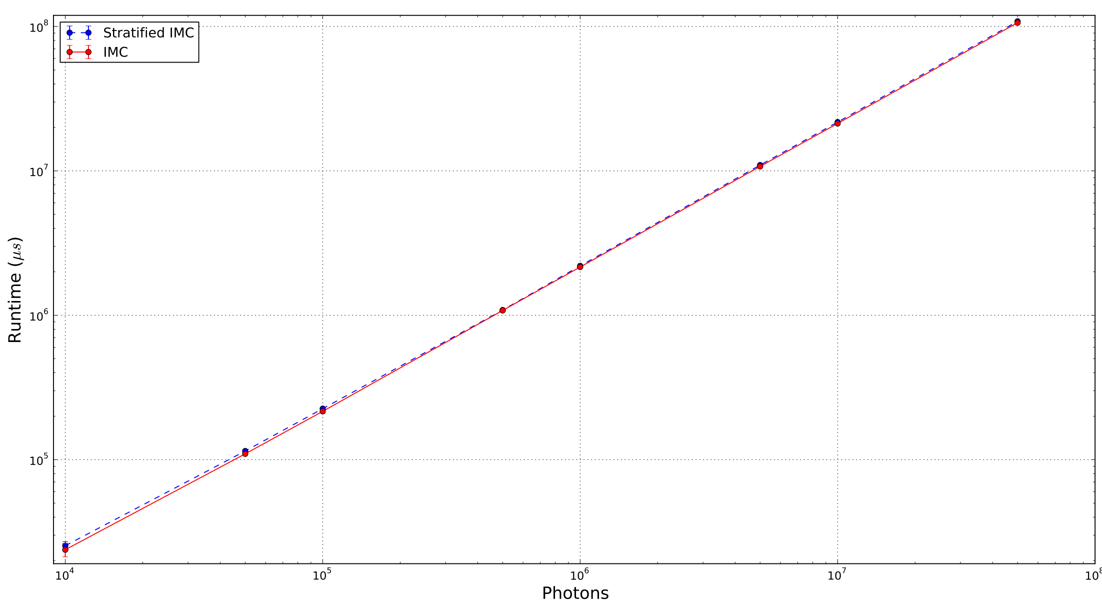

Fig. 3. Runtime vs. number of photons for a purely absorbing infinite medium problem at equilibrium after one time step

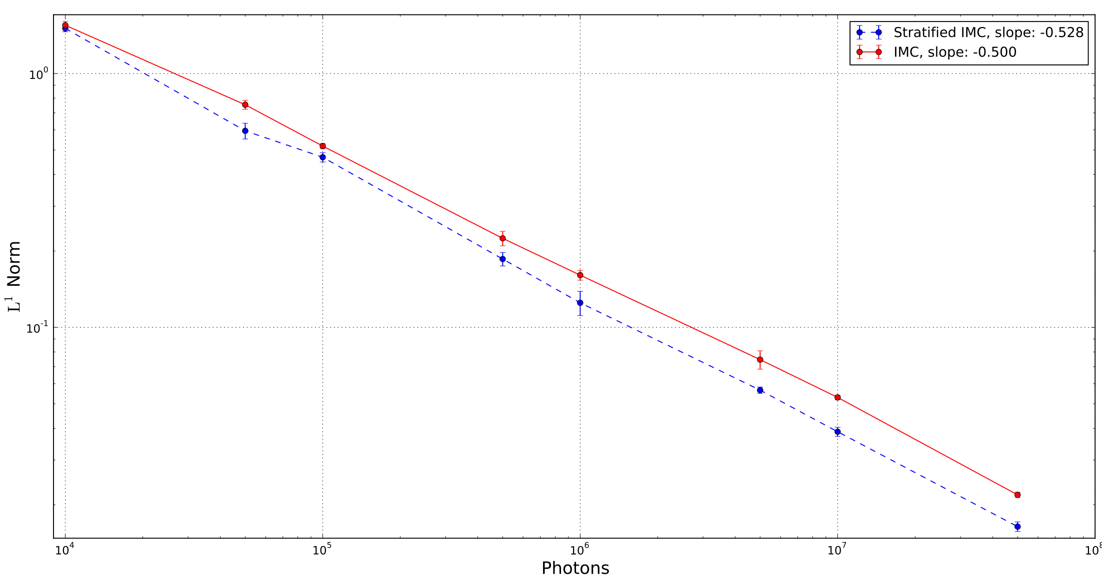

Fig. 4. Error vs. number of photons for an infinite medium problem with effective scattering at equilibrium after one time step