Improved Convergence Rates in Implicit Monte Carlo Simulations Through Stratified Sampling

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Alex Long and Ryan McClarren

Texas A&M University

Abstract

The Implicit Monte Carlo (IMC) method solves Thermal Radiative Transport (TRT) 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.

Overview

There are several methods of Monte Carlo Integration

Functions can be integrated by a Monte Carlo method. The error of the integral is

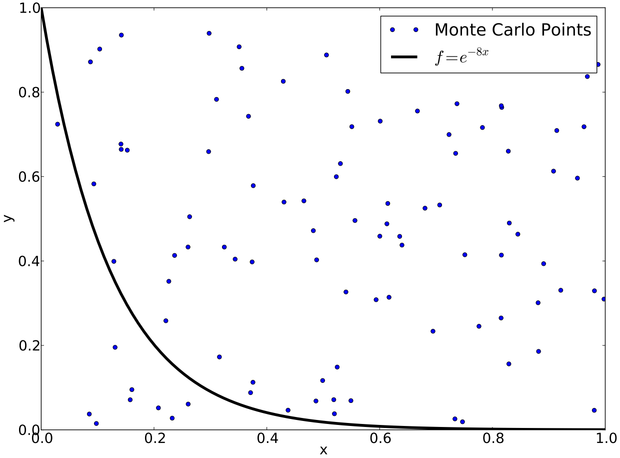
$$\epsilon \cong \frac{\sigma_1^2}{N^{1/2}},$$

where N is the number of samples. There are alternate methods that seek to reduce σ_1^2:

- Importance Sampling: More samples where function is large
- Stratified Sampling: The space is divided into strata and points are sampled in each of the strata
- Latin Hypercube Sampling: Further stratification for N samples–use N bins in each dimension

Monte Carlo Integration–Standard

Integrating the function $f(x) = e^{-8x}$, over $x = (0, 1)$. $N = 100$, $\mathrm{Error} = 0.028$



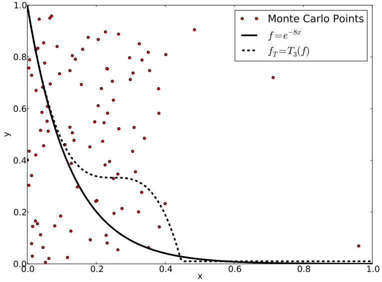
Importance Sampling

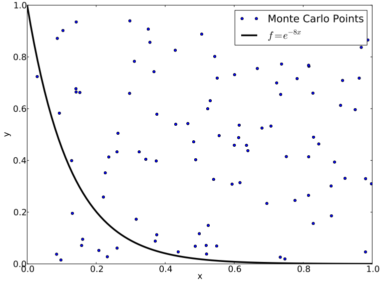
Sample from a function, $\tilde{f}(x)$, that's similar to the exact function. The integral is obtained by using (from Kalos and Whitlok):

$$G = \int \frac{g(x)f(x)}{\tilde{f}(x)} \tilde{f}(x) dx \tag{1}$$

- More points where the function is larger
- Analytic solution of ODE to sample emission in time
- For IMC, difficult to reduce variance in both variables

Integrating the function $f(x) = exp^{-8x}$ over $x = (0,1)$ with $N = 100$. With importance sampling, $\overline{\text{Error}} = 0.00625$. Without importance sampling, $\overline{\text{Error}} = 0.028$.





Stratified Sampling

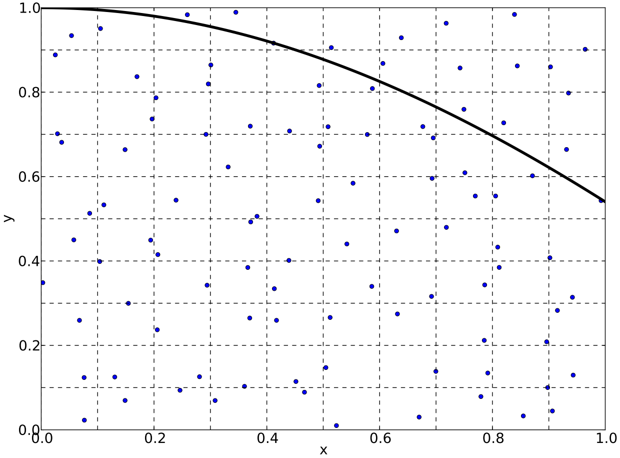
Represent as much of phase space as possible with a finite number of samples. Ideally, the number of desired integration points should be equal to the total number of strata.

$$N_s = N_{bins} = x_b y_b z_b \mu_b \phi_b t_b. \tag{2}$$

- Mean squared error is $O\left(N^{-(1+2/D)}\right)$ [1], where D is the number of dimensions that are stratified and N is the number of integration points
- Some strata end up being reused
- Scattering reduces improvements
- Potential for smooth memory access

Stratified Sampling

Integrating the function $f(x) = cos(x)$, over $x = (0, 1)$. $N = 100$, $\mathrm{Error} = 0.008529$



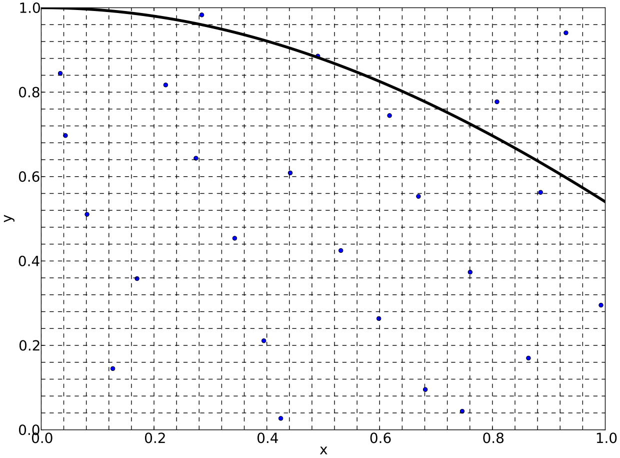
Latin Hypercube Sampling

Divide each dimension into N strata and place the integration points such that each discrete bin is only used once. The algorithm can be set to increase the spacing between points.

- Very computationally expensive to produce points
- Sampling pattern is not unique
- Scattering reduces improvements

Latin Hypercube Sampling

Integrating the function $f(x) = cos(x)$, over $x = (0, 1)$. $N = 25$, $\mathrm{Error} = 0.00147$



The Implicit Monte Carlo method solves TRT problems

- Thermal Radiative Transfer (TRT) describes interaction of matter and radiation fields
- In 1971 Fleck and Cummings publish a method for solving the TRT equations via Monte Carlo
- Fleck and Cummings method is called Implicit Monte Carlo (IMC)
- Source term is linearized
- IMC is not actually implicit

The Thermal Radiative Transfer (TRT) Equations

The familiar TRT equations, without scattering:

$$\frac{1}{c}\frac{\partial I(x,\nu,\Omega)}{\partial t} + \Omega \cdot \nabla I(x,\nu,\Omega) + \sigma_a(\nu) I(x,\nu,\Omega) = \sigma_a B(\nu, T), \quad (3)$$

$$\frac{\partial U_m(x, T, t)}{\partial t} = \int_0^\infty \int_{4\pi} \sigma_a I(x,\nu,\Omega)\, d\Omega\, d\nu - \int_0^\infty \sigma_a B(\nu, T)\, d\nu. \quad (4)$$

In frequency integrated problems (grey or "one group" in neutronics terminology), the IMC method is equivalent to linearizing the Planckian emission term with a Taylor series expansion:

$$\int_0^\infty \sigma_a B(\nu, T^{n+1})\, d\nu \approx \int_0^\infty \sigma \left(B(\nu, T^n) + \frac{\partial B}{\partial T}\frac{\partial T}{\partial t}\Delta t \right) d\nu \quad (5)$$

The IMC equations introduce effective scattering

After linearizing, an expression for U_r^{n+1} is used in the radiative energy balance. This leads to the IMC equations:

$$\frac{1}{c}\frac{\partial I}{\partial t} + \Omega \cdot \nabla I + \sigma_a(\nu) I = f \sigma_a B(\nu, T) + (1-f) \int \int \sigma_a I \, d\Omega' \, d\nu', \quad (6)$$

$$\frac{\partial U_m(x, T, t)}{\partial t} = \int_0^\infty \int_{4\pi} f \sigma_a I \, d\Omega \, d\nu - f \int_0^\infty \sigma_a B(\nu, T) \, d\nu. \quad (7)$$

Here f is usually referred to as the Fleck Factor:

$$f = \frac{1}{1 + \sigma_a c \Delta_t \frac{4aT^3}{cV}} \quad (8)$$

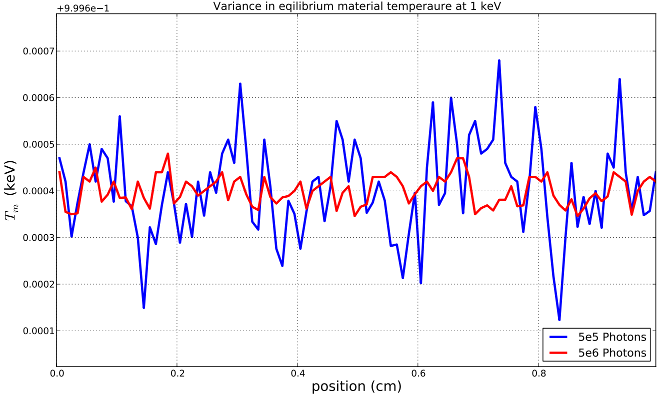
A simulated photon has a weight equal to its energy

- Thermal Radiative Transfer is a function of 7 independent variables
- Simulate the life of a “fauxton”: a group of particles with the same frequency representing some amount of the total energy in the problem
- User-specified number of photons are created that represent the energy in the radiation field.
- In IMC, the energy and frequency of a particle are not the same!
- A simulated photon is a group of photons of frequency, ν, having total energy E
- The energy of a particle is its weight

Variance is there, you just have to look close enough

Because IMC uses random numbers to sample phase space, material temperature and radiative intensity will have an associated variance

- Number of simulated particles differ by a factor of ten in the two lines below (problem used 100 zones):



Overview

Can sampling the space more effectively reduce variance appreciably?

Variance is undesirable: it can seed instabilities in coupled physics.

- TRT is a global problem
- Error can be reduced by running more particles, but it's $O\left(\sqrt{N}\right)$
- Reduce variance by using existing samples more effectively
- The future is less memory per core
- Trading memory for flops–generating sampling pattern vs. additional photons

Create a stratification pattern in each cell

The FINMCOOL IMC code, developed by students at Texas A&M University was used to test stratified sampling methods.

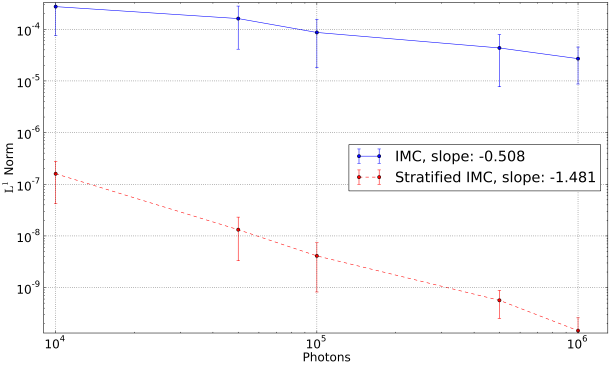
- In each cell, create strata using standard or LHS method
- Standard stratification–inexpensive, but samples are reused
- LHS stratification–very expensive, all samples independent

Overview

0D IMC problem at equilibrium

IMC holds equilibrium solution but will oscillate around it due to noise.

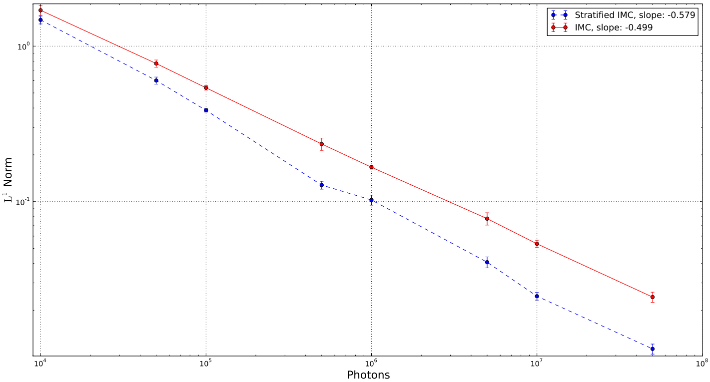
- One dimension, time
- Formula predicts $O\left(N^{-3/2}\right)$ error convergence
- In 0D, Stratification and LHS are the same



Infinite Medium

Also at equilibrium, spatial zones are introduced. $\Delta t = 0.1\mathrm{ns}$

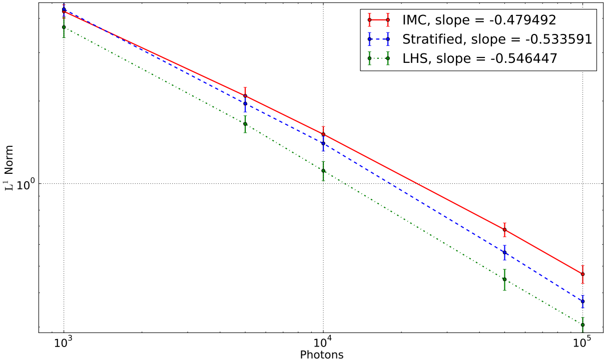
- 6 dimensions
- Formula predicts $O\left(N^{-2/3}\right)$ error for stratified



Infinite Medium–LHS Comparison

Also at equilibrium, spatial zones are introduced. $\Delta t = 0.1\mathrm{ns}$

- 6 dimensions
- Formula predicts $O\left(N^{-2/3}\right)$ error for stratified
- At around 100000 photons, LHS photon $\approx$ 2.8 standard photons



Infinite Medium–FOM Comparison

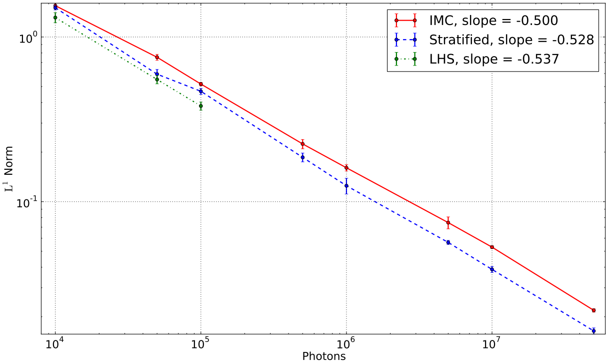
Figure of merit comparison, where $\mathrm{FOM} = \frac{1}{t\sigma}$.

Method	Photons	Run Time (s)	Error	FOM
Stratified	5×10^7	108.53	0.0069	1.335
LHS	5×10^4	87.92	0.447	0.025
Standard	5×10^7	106.16	0.01337	0.704

Infinite medium with scattering

Higher temperature reduces Fleck factor and introduces more effective scattering.

- 6 dimensions
- $\sigma = 1.0\ \mathrm{cm}^{-1}$, $f = 0.79$



Overview

Conclusions and future work

Conclusions

- Stratification can improve the FOM on optically thin problems
- More scattering makes angle stratification unimportant
- Latin Hypercube Sampling is better than standard stratification but very computationally expensive

Future Work

- Extend to smooth emission IMC of Trahan and Gentile [3]
- Other stratification strategies for problems with scattering
- Test cache misses with and without stratification

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