VARIANCE REDUCTION TECHNIQUES FOR IMPLICIT MONTE CARLO SIMULATIONS

An Undergraduate Research Scholars Thesis

by

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ABSTRACT

Variance Reduction Techniques for
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The Implicit Monte Carlo (IMC) method is widely used for simulating thermal radiative transfer and solving the radiation transport equation. During an IMC run a grid network is constructed and particles are sourced into the problem to simulate the transport of energy in the form of radiation. Particles that reach the end of a time step without losing their entire energy are moved to "census" and will continue in the next time step. In order to reduce the variance of the solution, a neutronics technique called "weight windows" is applied, which allows for a greater number of particles to reach the census. With a larger number of particles in each grid, obtaining good statistics becomes much more probable. Along with weight windows, two other techniques called "Roulette" and "Analog" are implemented to remove excess particles from the problem and reduce computational time. The implementation of these techniques should reduce the total variance of the solutions obtained using IMC and increase the efficiency of Monte Carlo particle simulations.

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CHAPTER I

AN INTRODUCTION TO IMPLICIT MONTE CARLO SIMULATIONS

The Importance of Computer Applications

In the field of nuclear physics, heat transfer and other processes can be obtained by either experimental investigation or by theoretical calculations. Experimental investigations are very reliable but are often expensive and impossible to accomplish. Instead, many researchers use theoretical calculations, which can include either analytical mathematical modeling or numerical mathematical modeling. Analytical calculations usually involve solutions to sets of differential equations. Unfortunately, there is only a small fraction of practical problems that can be solved analytically. Fortunately, numerical methods are continuously being developed that can simulate almost any practical problem. Numerical methods use algebraic equations opposed to differential equations, which makes them powerful and widely applicable. The advantages of using numerical methods opposed to experimental methods include lower costs, faster simulations, the ability to obtain complete information, and the ability to simulate realistic and ideal conditions. Although, the uncertainty of a specified mathematical model limits the usefulness of a numerical computation. Thus, it is necessary to reduce the variance in numerical simulations so that computer simulations become more applicable.

How Monte Carlo methods were discovered

In 1946, Stan Ulam began to question what the chances were of a solitaire game laid out with 52 card ending successfully. After much time was spent attempting to apply combinatorial calculations, Ulam began to wonder whether or not there was a more practical method than abstract thinking. Ulam "immediately thought of problems of neutron diffusion and other questions of mathematical physics" and described the idea to John von Neumann [1]. An intrigued Neumann wrote to Robert Richtmyer who "concluded that the statistical approach

was very well suited to a digital treatment"[1]. Richtmyer then outlined in some detail how that method could be used to solve neutron diffusion and multiplication problems in fission devices. Years later in 1963, Fleck published on using Monte Carlo as a means of solving the equations of thermal radiative transfer.

The Basics of Implicit Monte Carlo Simulations

"In Monte Carlo calculations the particle tracks or histories are generated by simulating the random nature of the particle interactions with the medium"[3]. As a particle interacts with the material medium, its experiences are tallied in various ways to yield quantities such as intensity, flux, and particle distributions. Monte Carlo calculations can treat very complex three dimensional configurations as well as treat energy, spatial, and angular dependences. This eliminates discretization errors, but variance can still be observed due to stochastic uncertainties. The accuracy of Monte Carlo calculations is roughly inversely proportional to the square root of the number of events contributing to some response. Thus, it is advisable to simulate a large number of neutron histories in order to increase the accuracy of the results.

Monte Carlo methods require the use of a pseudo random number generator to simulate the physical phenomena associated with nuclear physics. The term "pseudo" comes from the fact that Monte Carlo methods do not use true random numbers. In actuality, an algorithm is developed which generates these "random" numbers and at some point the generated numbers will begin to cycle and repeat themselves. During Monte Carlo simulations, random numbers are used to determine a particle's position, angular direction, distance to collision, and type of collision. In 1971, Fleck and Cummings introduced "the concept of effective scattering, wherein a fraction of the radiative energy absorbed is instantaneously and isotropically reradiated in a manner analogous to a scattering process"[2]. This method that Fleck and Cummings developed is called Implicit Monte Carlo.

A Brief Overview of Variance Reduction Techniques

Monte Carlo simulations have been used for a decades to simulate real world phenomena. These simulations rely on repeated random sampling and tallies to simulate the random nature of particle interactions. Due to the random positioning of particles and the use of tallies, the solution obtained from the simulation will have an associated variance. Variance reduction techniques for Monte Carlo neutron transport problems have previously been researched and are currently understood. On the other hand, Implicit Monte Carlo photon transport problems still need the addition of variance reduction techniques in order to achieve accurate global solutions.

In order to reduce the variance, it is desired to achieve a more uniform distribution of particles. To do this "one must either increase the number of particles simulated, or modify the Monte Carlo procedure in such a way that (i) the probability of particle survival is increased in low populated regions and (ii) the mean solutions do not become biased" [4]. The goal is to increase the number of particles that will contribute to a desired response (i.e., flux, dose, reaction rate, etc.). Accomplishing this will enable the contributing distribution to become closer to the mean value. Some standard variance reduction techniques are as follows:

- Absorption Suppression
- Splitting and Russian Roulette
- Forced Collision
- Source biasing

The following chapter will go into further detail of these variance reduction techniques and the techniques I developed as an undergraduate research scholar. It should be noted that not all of the above techniques were explored during my research.

CHAPTER II

MONTE CARLO WEIGHTED SAMPLING

In traditional Monte Carlo applications, the main objective is to calculate a mean value:

$$\bar{x} = \int x f(x) dx,$$

where $\bar{x}$ is a desired response of the particle history and $f(x)$ is the probability density function being sampled. In nontraditional Monte Carlo applications, a modified probability density function, $\tilde{f}(x)$ is sampled and weighted by $w(x)$, where:

$$w(x) = \frac{f(x)}{\tilde{f}(x)}.$$

The use of weighted sampling preserves the mean value of $\bar{x}$, which can be written as:

$$\bar{x} = \int x w(x) \tilde{f}(x) dx.$$

It is very important to understand this concept in order to successfully apply variance reduction techniques in a way such that an unbiased estimate of the mean is maintained.

Explanation of Traditional Variance Reduction Techniques

Absorption Suppression

During absorption suppression, a particle's history is not terminated upon absorption. Instead, the weight of the particle is reduced by replacing the current particle's weight by the following:

$$w_{new} = w_{old} * \left(1 - \frac{\Sigma_a}{\Sigma_t}\right).$$

With this technique implemented, the only way for a particle's history to be terminated is through leakage, which leads to an undesired increase in computational time. Plus, if the dimensions of the problem being ran are large, then inefficient sampling will take place. At some point the weight of the particle will become so low that it will no longer have any significant contributions to the desired response. To counteract this characteristic other techniques can be used in conjunction with absorption suppression.

Splitting and Russian Roulette

If a particle's weight becomes small and unimportant (i.e. during absorption suppression), a technique called Russian Roulette can be implemented to terminate these particles, which in turn will decrease the computational time. Russian Roulette works by first generating a random number and determining whether that number is greater or less than a specified "probability of survival". If a particle loses roulette, its history will be terminated, and the remaining energy that the particle contained will be placed into a "bank" for a short period of time. On the other hand, if a particle wins roulette, it will be given some, if not all, of the energy contained in the "bank", and its weight/importance will be increased by the same relative amount.

Alternatively, if a particle's weight becomes extremely large, it is advantageous to split the particle into additional particles. This leads to better statistics due to the increase in particles contributing to the response. Upon applying this technique, the original weight of the particle being split will be distributed evenly to the additional particles that were created.

Forced collisions

In some instances the distance between collisions needs to be shortened in order to obtain a significant amount of contributions to the desired response. To help explain this, imagine if a problem contained a certain material that lead to an extremely large mean free path. Very few particles would collide with this material and contribute to the mean, thus the particles must be "forced" to collide and interact with the medium. This is accomplished by splitting a particle into two smaller weight particles where the first passes through the material and the second is forced to collide.

Source biasing

During source biasing, a parameter is set upon creation of the particles in such a way that regions containing particles with large weights (without source biasing) will source additional particles and vice versa for regions containing particles with small weights. This method ideally creates more additional particles in regions with low responses and fewer additional particles in regions with high responses.

Initial IMC Variance Reduction Methods

Two different approaches have been researched thus far to reduce the total variance in IMC solutions. Initially, the following three methods were explored: source biasing, a method dubbed "analog", and splitting/Russian Roulette. A weight window was introduced into the software which restricted particles to have weights equal to the weight window center. If a particle contained a weight larger than the upper bound of the weight window then the particle would be split into additional particles, and if a particle contained a weight lower than lower bound of the weight window the particle would undergo either Russian Roulette or the analog method. As these methods were explored, the current energy of the particle was taken to be the weight and the weight window center was set to the radiative energy of the particles current zone.

During analog, the distance to the next collision was taken into account instead of the distance to the next scattering event. If, based on a random draw, the next event was an absorption, then the particle died and it's energy was deposited into the material. This technique increases the probability of an interaction with the medium, which subsequently removes the particle from the problem and deposits its energy into the medium.

During Roulette, any particle below the weight window is either killed or promoted to the radiative energy level with probability equal to the ratio between the current particle energy and the radiative energy of the current cell. In order to conserve energy, a "bank" is introduced that is exclusive to each zone. When a particle is terminated, its energy is deposited into the "bank" and at the end of each time step the bank is either deposited into the material or attributed to a census particle. Effectively the Roulette technique combines low energy particles into single particles with the desired energy, which in turn should decrease computational time.

Source biasing was another technique explored that failed to give meaningful solutions. In this process the number of particles created in each zone was determined in such a way that each particle contained an energy equal to the radiative energy of that zone. This method lead to large decreases in computational time, but unfortunately the variance in the solutions increased.

Current IMC Variance Reduction Methods

The current techniques that are being implemented/explored are the analog method, and splitting/Russian Roulette. Unlike the previous weight window center, the current weight window center is being set to the zone's intensity from the previous time step. Additionally, the current particle's energy is no longer taken to be the particle's weight. Instead, each particle is created with a weight equal to the weight window center of that zone (making source biasing unnecessary). Creating a weight parameter separate from the energy parameter is an important characteristic of the current IMC variance reduction approach. This

addition keeps the weighted importance dimensionless and allows one to use an quantity as their weight window center (i.e. material temperature, energy density, path length, etc.).

In addition to the particle weight changes, when a particle is promoted during Roulette its energy is increased by the inverse of the probability of killing the particle. Although, if the bank does not contain enough energy, then the entire bank energy is given to the particle, and the weight of the particle is increased by the same relative amount. There have been no changes made to the analog method.

There is also one other technique that has been implemented apart from "Weight Windows". As a particle enters into a new zone a function will determine, based off of its current energy, the maximum rise in material temperature that could occur. If the rise in temperature is higher than a certain percentage decided by the user, then that particle will split into additional particles and its energy will be distributed accordingly. This function has been tested to be correct, but as the number of particles increases and the size of the zones decrease, the use of this method becomes unnecessary.

The following chapter will discuss the results obtained using the current variance reduction techniques.

CHAPTER III

RESULTS/CONCLUSION

Initial Method Solutions

Marshak Wave Solutions

The initial variance reduction methods implemented proved to be very effective and efficient. To compare effectiveness, solutions were obtained by simulating a 1-D Marshak wave problem. During these simulation, the initial temperature of the material in the Marshak wave problem is set to 0.001 keV with a 1.0 keV source on the left plane. In addition, an "accurate" solution was found by running the simulation with one million particles without the use of variance reduction techniques. Figure (III.1) below shows the material temperatures obtained using each of the techniques. The solutions were obtained using only 5000 particles and proved to be pretty accurate in comparison to the correct solution. In addition, the variance reduction techniques required much less computational time.

Figure (III.2) is a plot of the number of photons that entered each zone. Without the use of weight windows, there is a high concentration of particles in particular areas of the problem. On the other hand, both Roulette and Analog allowed for a more even distribution of particles, which in turn increases the probability of receiving good statistics.

Figure (III.3) introduces a Figure of Merit(FOM) as a function of distance that was used to compare the efficiencies between the different IMC methods. Both the variance and the computational time are included in the FOM, which can be defined by the equation below. In the equation, σ is the deviation between the solution obtained and the "accurate" solution.

$$\text{FOM} = \frac{1}{\sigma^2 * \text{time}}$$

In this case it is demonstrated that the analog method is the most efficient. The solutions obtained using Russian Roulette, analog, and no variance reduction took approximately, 100.6, 137.1, and 1600.2 seconds, respectively. Although, the solution obtained using the analog method contained the least amount of deviance from the accurate solution.

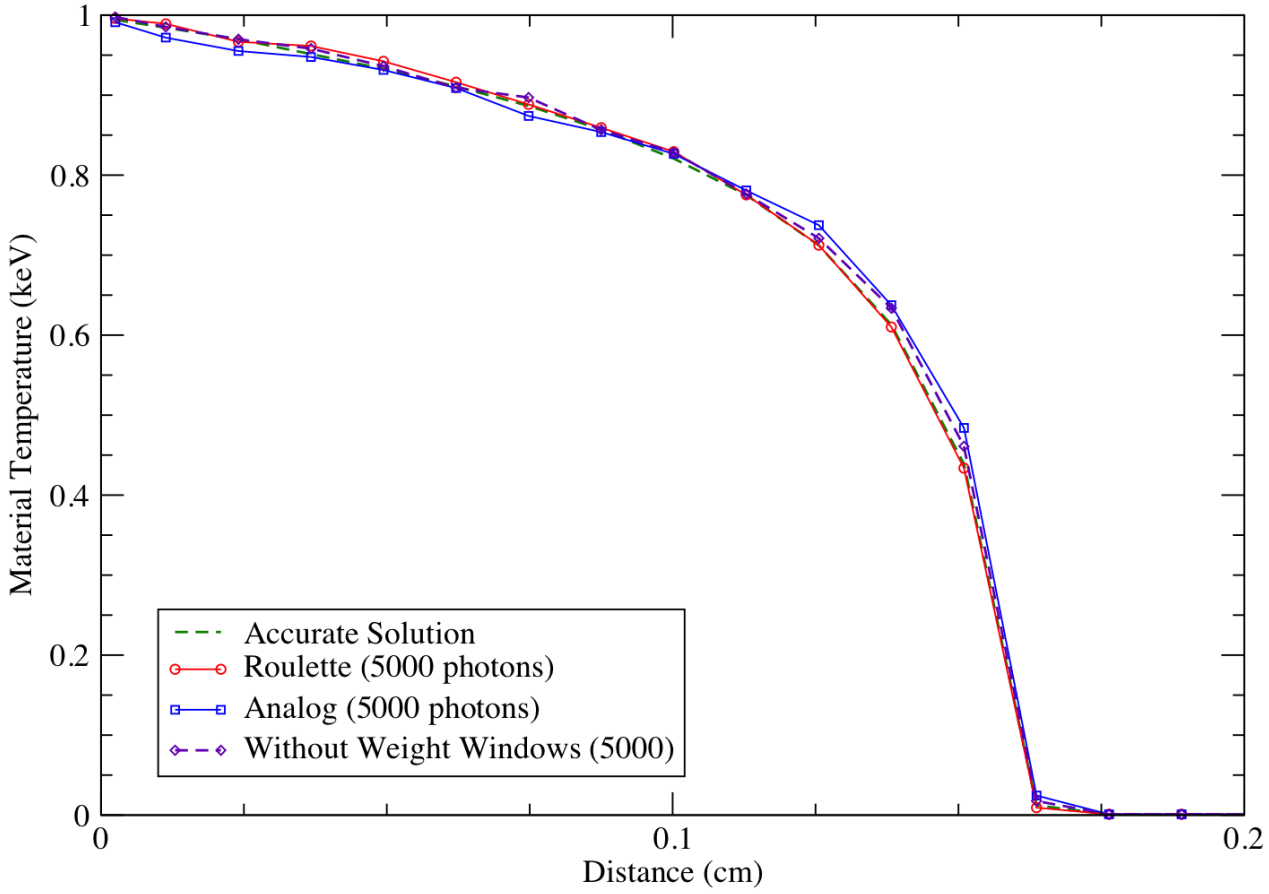

Fig. III.1. 1-D Marshak Wave Results

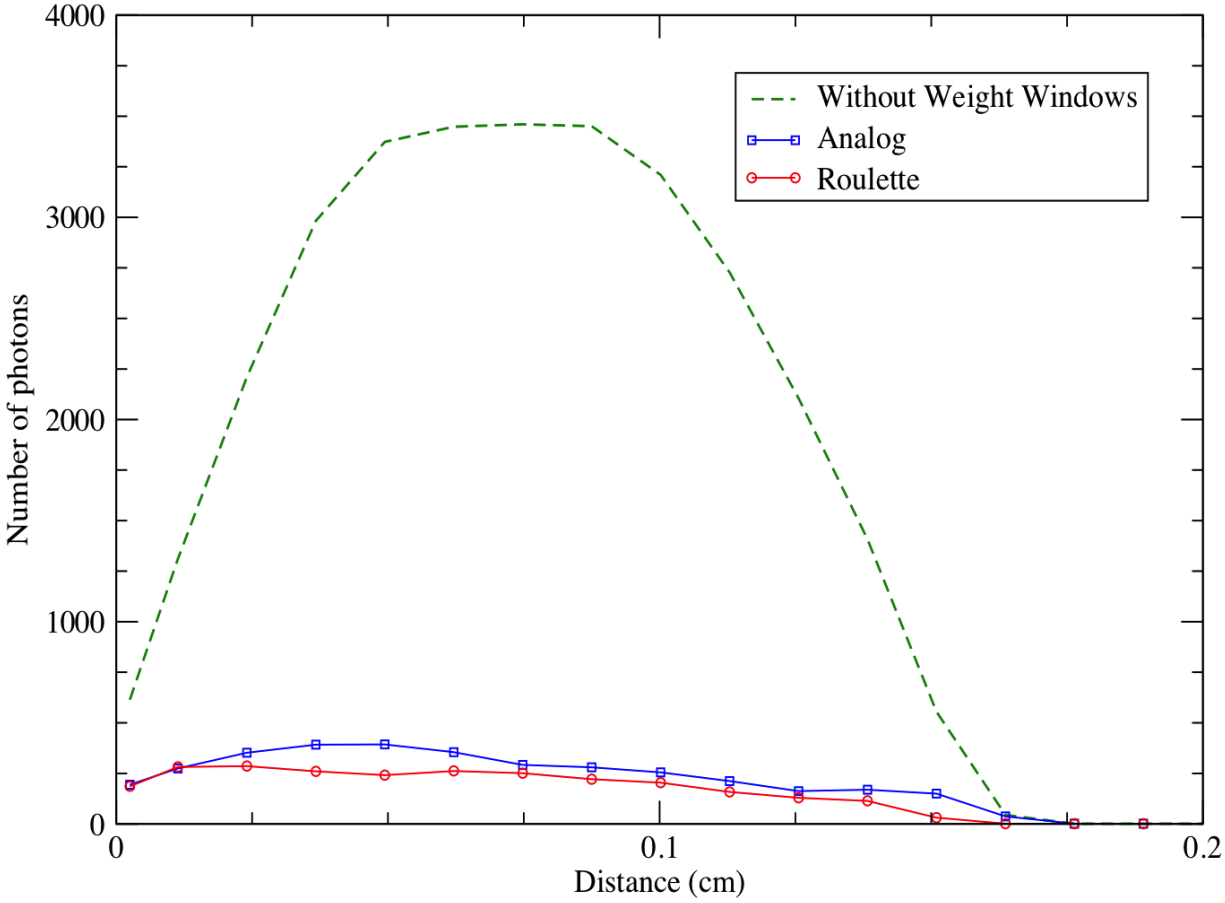

Fig. III.2. 1-D Marshak Wave Zone Photons

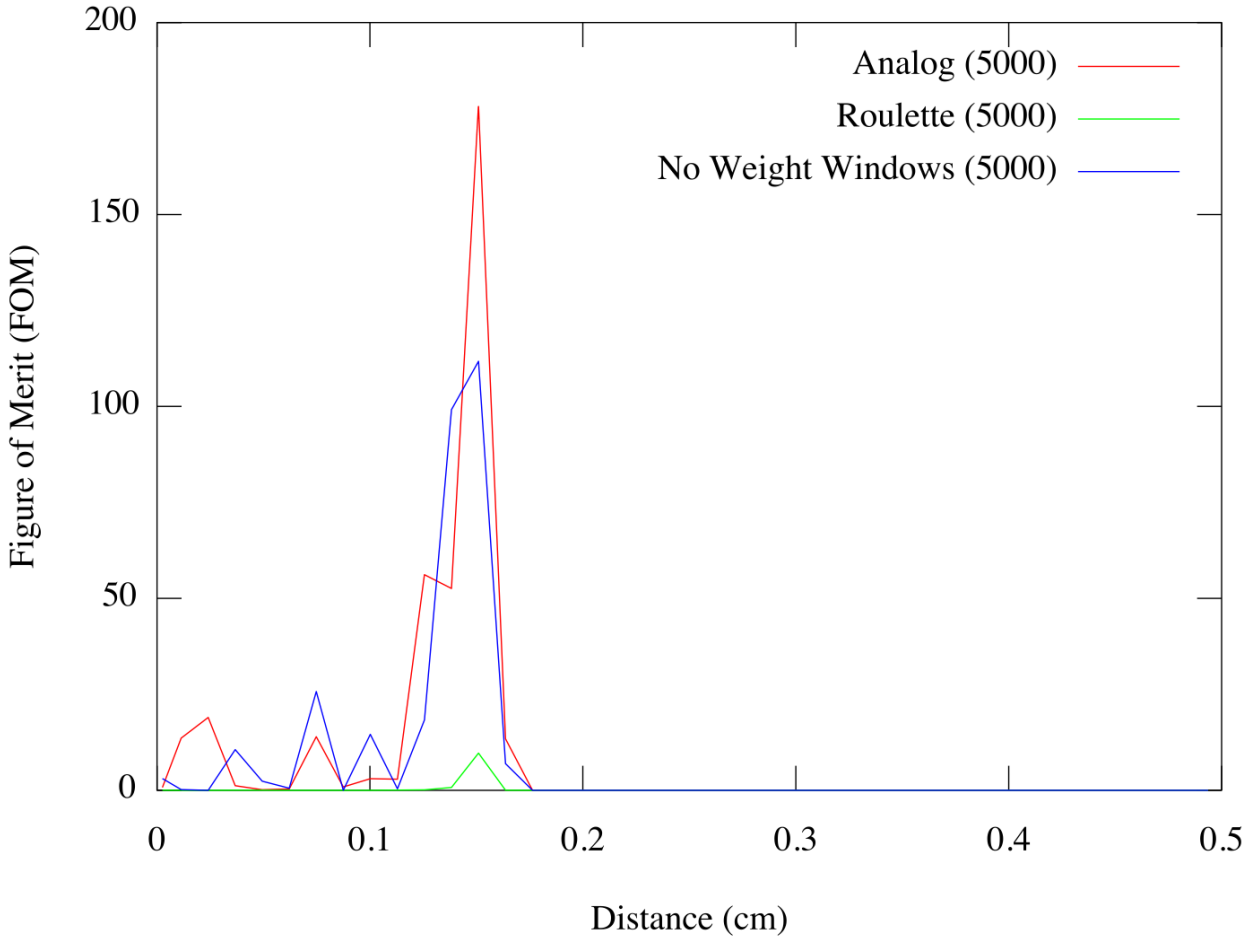

Fig. III.3. 1-D Marshak Wave Figure of Merit

Tophat Simulations

Furthermore, simulations were ran on a 2-Dimensional "tophat" problem to determine the applicability of the variance reduction methods on problems with larger dimensions. The tophat schematic is shown by FIg. (III.4) and contains an incoming source of radiation originating from the left plane of the optically thin portion. The material temperature of all the solutions were nearly identical, but the number of photons in each zone was determined to be much more uniform with the use of the variance reduction methods. Figures (III.5) and (III.6) compare the number of photons in each zone found using variance reduction vs. without variance reduction. Unlike the solutions found for the 1-D Marshak wave problem, the roulette method was determined to be the most ideal due to its ability to uniformly distribute particles.

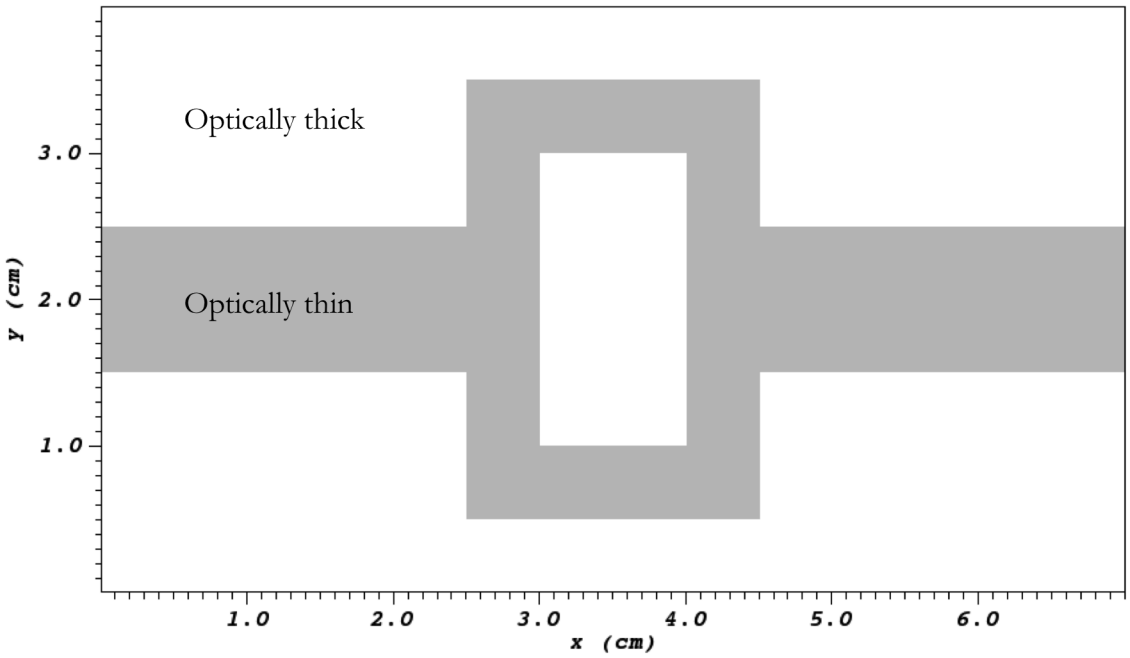

Fig. III.4. 2-D Tophat schematic

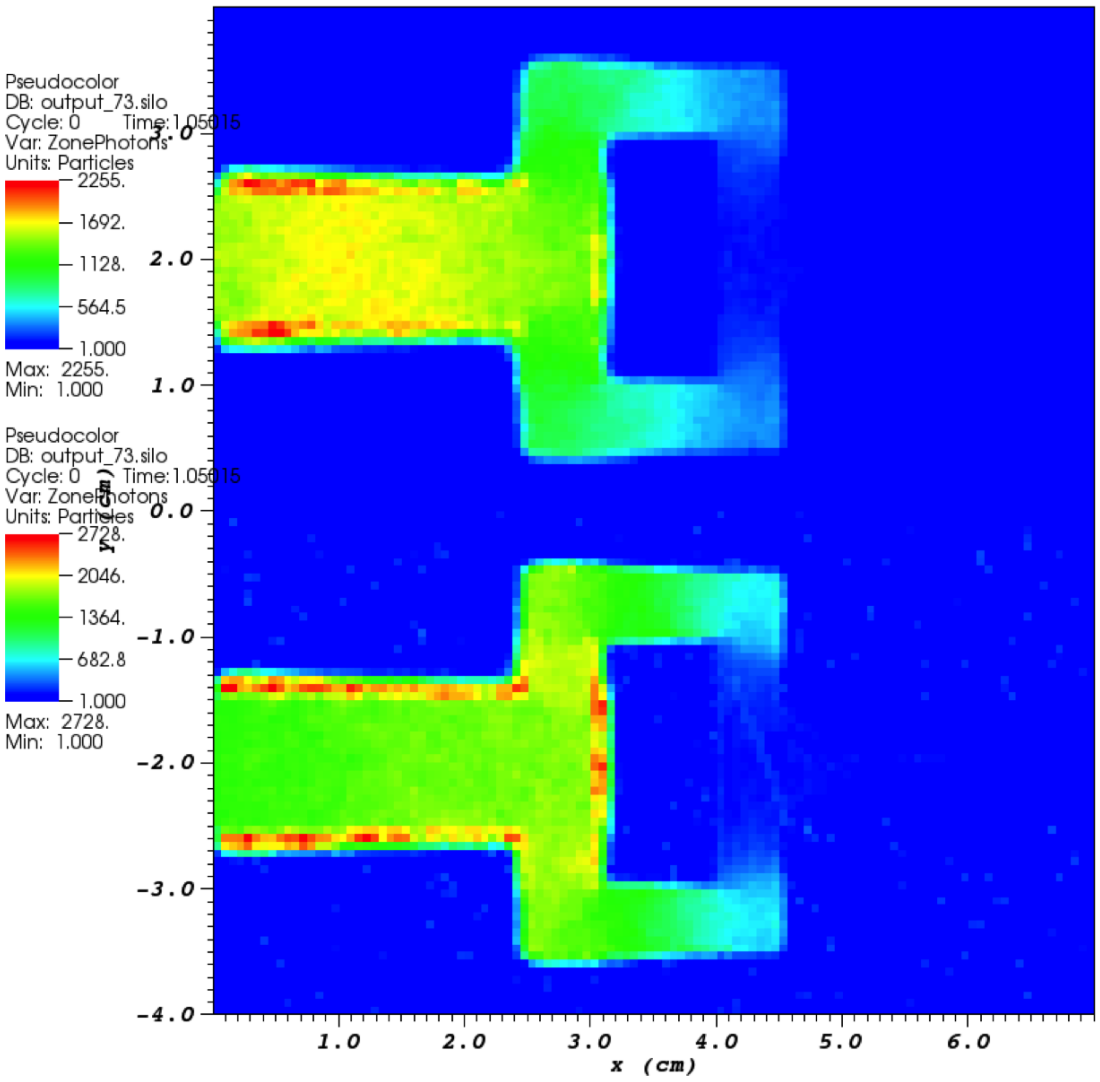

Fig. III.5. Zone Photons: No Variance Reduction (Top) vs. Roulette (Bottom)

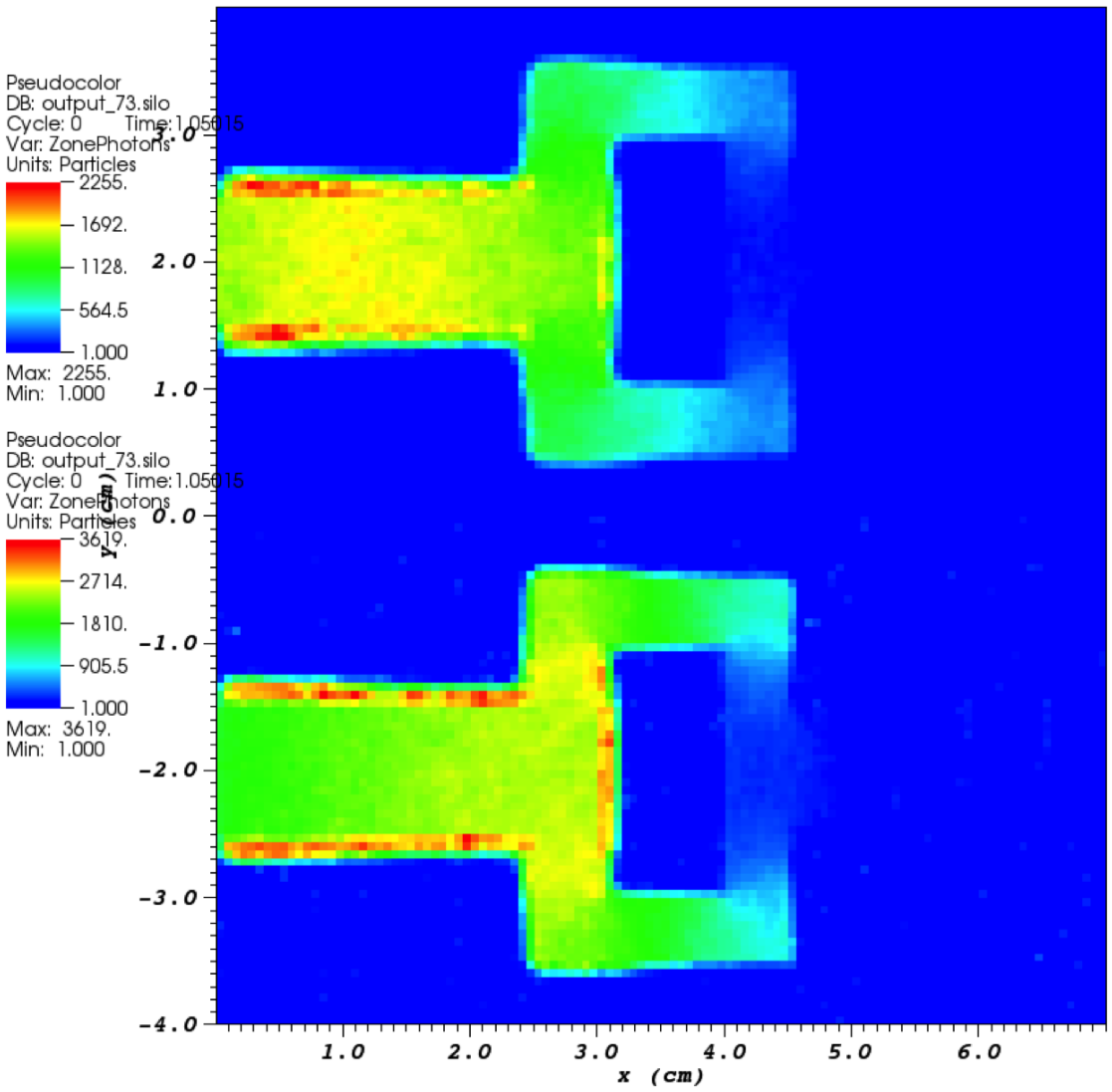

Fig. III.6. Zone Photons: No Variance Reduction (Top) vs. Analog (Bottom)

Current Method Solutions

Marshak Wave Solutions

With the new weight implementation, the analog method has increased the computational time by an unacceptable amount. Due to this, the Russian Roulette was the only method worth further exploration. Russian Roulette coupled with weight windows has proven to be a very efficient method. This can be seen from the 1-D Marshak Wave results depicted in Fig. (III.7). This figure illustrates that using weight windows coupled with Roulette gives more accurate solutions than without variance reduction. Additionally, the simulation ran without variance reduction took 5203 seconds opposed to only 881 seconds with variance reduction. In other words, the solution obtained using variance reduction was more accurate and 83% faster! It is clear from the results that Russian Roulette is much more efficient than not using variance reduction.

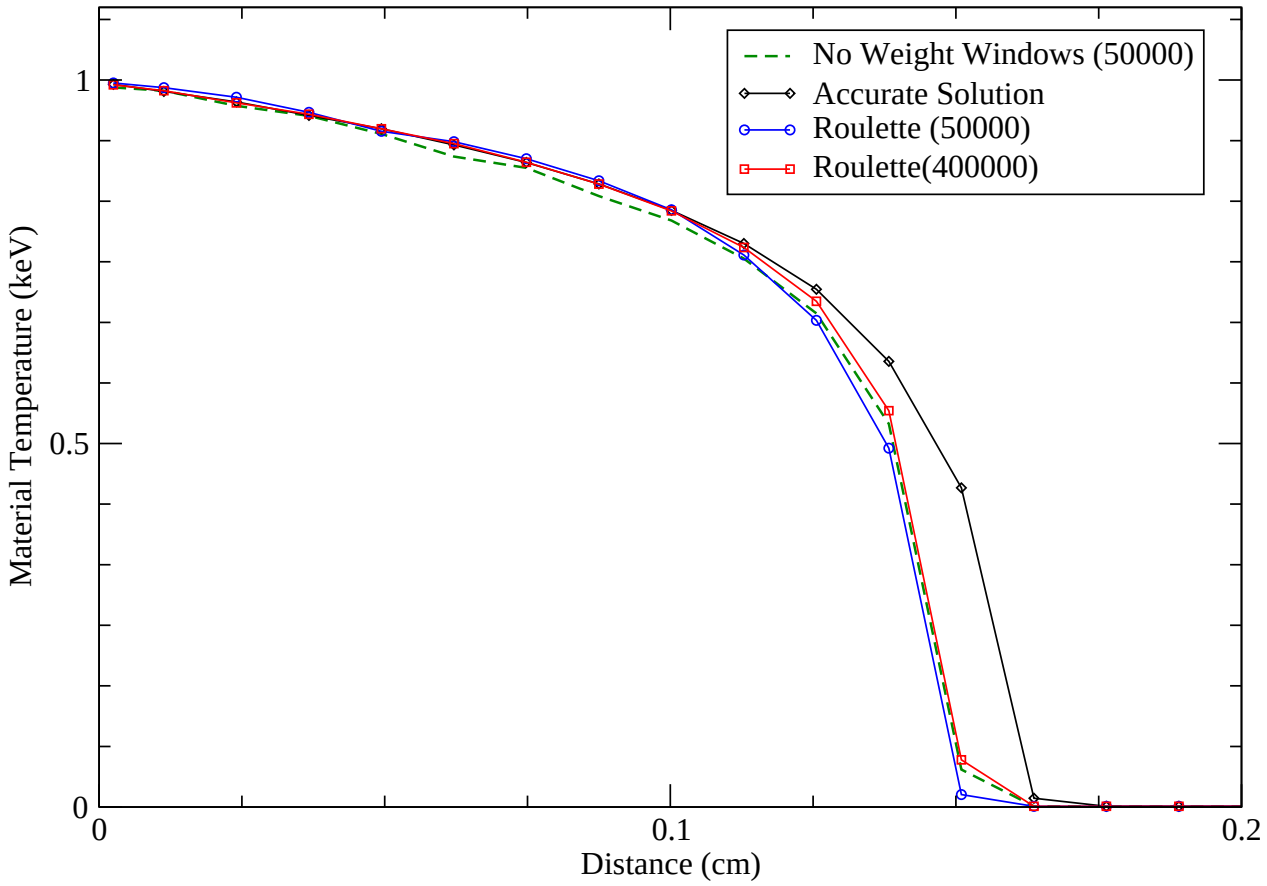

Fig. III.7. 1-D Marshak Wave Results

Tophat Solutions

The tophat solutions found using the new weight parameter have been found to be not as efficient. Although the computational time is practically halved with the use of variance reduction, the solution has been observed to be inaccurate. Currently, there is too much energy being deposited into the material during Russian Roulette. As seen in Fig. (III.8), this is causing hot spots to occur in the solution which is inaccurate. Creating additional census particles and giving them the excess "bank" energy will likely counteract this issue. Figure (III.9) depicts the number of particles that are in each zone. As desired, there are more particles that contribute to the response in the solutions with variance reduction. This will theoretically lead to more accurate solutions given that the hot spot issue is resolved.

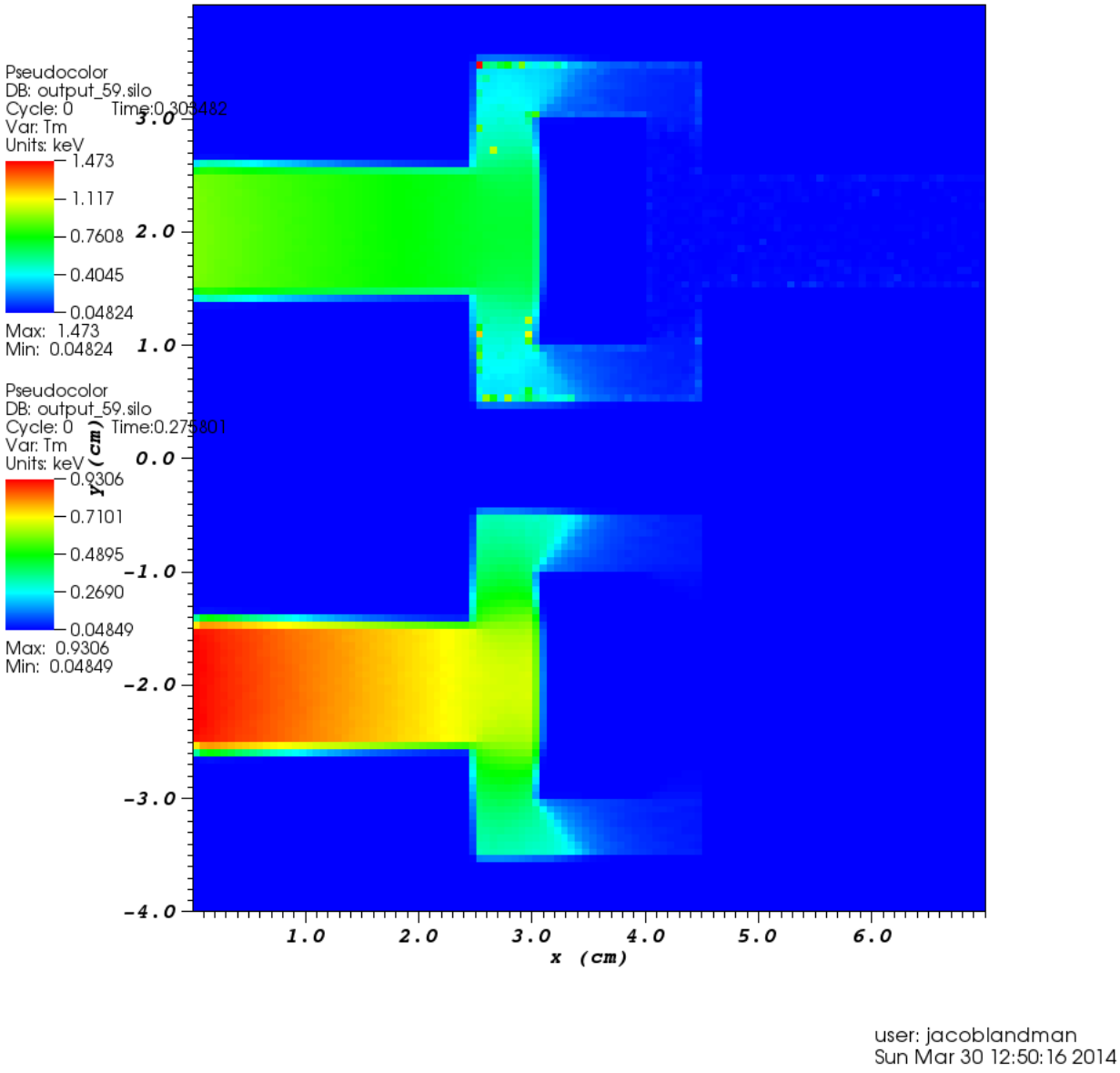

Fig. III.8. Material Temperature: Roulette (Top) vs. No Variance Reduction (Bottom)

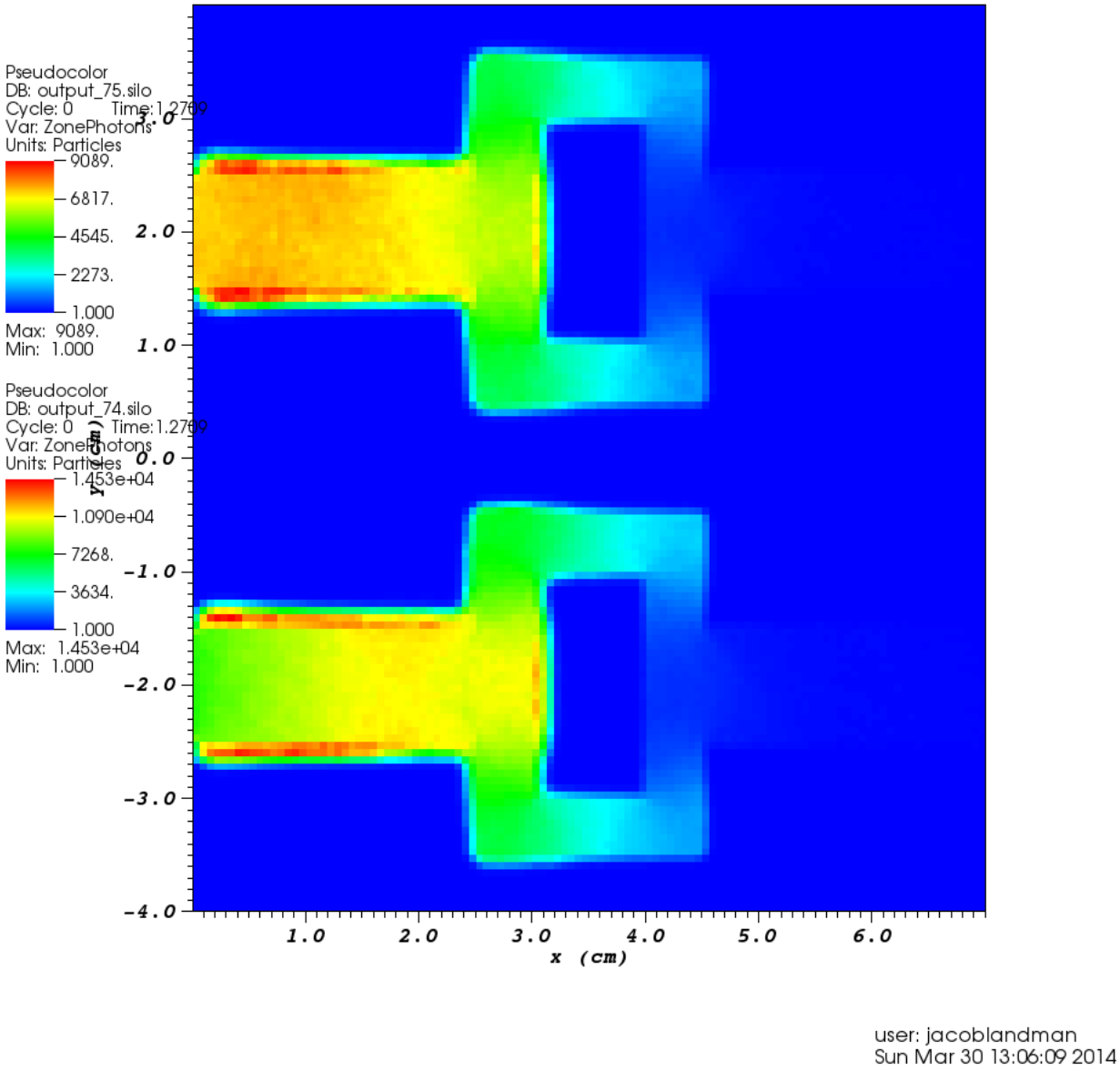

Fig. III.9. Zone Photons: Roulette (Top) vs. No Variance Reduction (Bottom)

Conclusion

In summary, two approaches were explored to reduce variance in Implicit Monte Carlo Simulations. The first approach attempted to use the current energy of the particle as a weight for weight window applications. This approach successfully reduced the amount of computation time by approximately 90% compared to solutions obtained without the use of variance reduction. The use of analog proved to be the most efficient to its ability to produce quick, accurate solutions.

The second approach utilized the addition of a "weight" parameter associated with each particle in the simulation. This addition theoretically allows any desired response to be used as the weight window center due to the lack of dependence on the particle's energy. In my study, the zone intensity was set to the particle weight and was used as the weight window center. As a particle went from high to low intensity zones, it would split into additional particles to improve the probability of obtaining good statistics. When a particle's weight became extremely low, it would undergo Russian Roulette, ridding the simulation of the useless particles. The method successfully reduced the error and decreased computational time in 1-D simulations, but more work is needed to improve the usefulness of these variance reduction methods with 2-D problems.

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