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QUASI-PHOTON MONTE CARLO ON RADIATIVE HEAT TRANSFER: AN IMPORTANCE SAMPLING APPROACH

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ABSTRACT

The radiative heat transfer phenomenon is a complex process with various events of absorption, emission, and scattering of photon rays. Moreover, the effect of a participating medium adds to the complexity. Existing analytical methods fail to achieve accurate results with all such phenomena. In such cases, brute force algorithms such as the Monte Carlo Ray Tracing (MCRT) or the Photon Monte Carlo (PMC) has gained a lot of importance. But such processes, even if they provide less error than analytical methods, are quite expensive in computation time. Moreover, there are various shortcomings with traditional PMC in effectively including the nature of the participating medium and high variance in results. In this study, a modified PMC is simulated for a one-dimensional medium-surface radiation exchange problem. The medium is taken to be CO (4+) band system, and the behaviour is modelled by Importance Sampling (IS) of the spectrum data for variance reduction. Furthermore, PMC with low-discrepancy sequences like Halton, Sobol, and Faure sequences, known as Quasi-Monte Carlo (QMC), was simulated. QMC proved to be more efficient in reducing variance and computation time. Effective IS included with QMC is observed to have a much smaller variance and is faster as compared to traditional PMC.

Keywords: Radiative Heat Transfer, Photon Monte Carlo, Importance Sampling, Quasi Monte Carlo, Low-Discrepancy sequences

1. INTRODUCTION

At high temperature, radiative heat transfer is the dominant mode of heat transfer. It is governed by various phenomena such as photon emission, absorption, and scattering. Molecules and atoms of the participating medium absorb the radiation energy. The solution to radiation transport in participating media may be obtained by solving the Radiative Transfer Equation (RTE),

$$\frac{1}{c} \frac{\partial I_\lambda}{\partial t} + \frac{\partial I_\lambda}{\partial s} = \kappa_\lambda I_{b\lambda} - \kappa_\lambda I_\lambda - \sigma_{s\lambda} I_\lambda + \frac{\sigma_{s\lambda}}{4\pi} \int_{4\pi} I_\lambda(\hat{s}_i) \phi_\lambda(\hat{s}_i, s_i) d\Omega_i \quad (1)$$

where, c is the speed of light, $\kappa_\lambda I_{b\lambda}$ represents the energy gained by emission, $\kappa_\lambda I_\lambda$ denotes the energy losses to absorption and $\sigma_{s\lambda} I_\lambda$, the redistribution of the energy by scattering. The last term on the right hand side of the equation accounts for the radiation scattered from other directions onto the surface. The analytical solution of this governing integrodifferential equation of radiative transfer is a complex process and possesses various shortcomings, more when the effect of participating medium and wavelength properties are taken into consideration. Although a generic formulation of such radiative transport problems can be modeled for a wide variety of problems with non-gray, non-diffusive surfaces, there is always a trade-off between simplicity and accuracy of the problem.

The common techniques for solving the mathematical models of radiative transfer generally rely on various degrees of approximation. The discrete ordinates technique approximates integrals over direction by a numerical quadrature technique, and the radiative intensity is assumed to be constant within each quadrature direction. The solution will approach exactness as the number of quadrature elements is increased. The P-N or spherical harmonics method describes the radiative intensity as an orthogonal infinite series expansion in terms of distance and angle and then truncates the series to a set that can be conveniently solved. There are essentially no exact analytical solutions available to the radiative transfer equation except for quite simplified choices of geometries and property variations.

Recently, solutions to complicated mathematical problems with statistical methods based on the randomization of naturally occurring phenomena have gained significant importance. In

radiative transport, the total radiative energy transferred is discretized into a number of energy packets, or photon bundles. These energy bundles are selected randomly to describe the emission, absorption, and scattering processes. This approach to radiative transfer simulations is guided by a Monte Carlo Ray Tracing (MCRT) algorithm. The method is known as the Photon Monte Carlo (PMC). PMC is a simple, yet powerful technique, to solve radiative transfer problems in complicated geometries with arbitrary participating medium. The method, on the one hand, increases the accuracy of estimation, and on the other hand, increases the computational cost. This Monte Carlo method is able to incorporate all important effects in a radiative transfer simulation without approximation, and this is its major attribute. Due to the stochastic nature of the method, the results inherently possess statistical behaviour. This can be a benefit in that the uncertainty in the results can always be determined.

The PMC method has been quite a significant topic since 1988. Howell [1] presented various strategies for performing Monte Carlo simulations and also the problems in radiative transfer that are studied based on such methods. Modest [2] in his work on backward ray-tracing algorithms, presented the Backward Monte Carlo simulations to counter arbitrary radiation sources, including point and plane sources. Wang and Modest [3] worked on the ray-particle interaction models based on various participating media particle representations. The spectral Line-By-Line model developed by them for the non-gray radiation analyses proved to be a benchmark for testing the accuracy of various radiative transfer algorithms.

The requirement of large computational power is a significant problem in the Monte-Carlo methods, and the accuracy is directly proportional to the number of rays tracked. With low numbers, such simulations generally provide high variances. Iwabuchi [4] presented an approach for variance reduction based on the local estimation method.

In various problems, the participating media — generally a gas, such as CO₂, CO, or H₂O — present complex emission and absorption spectra. Recently, various new approaches are proposed to include the participating media into the effective heat transfer simulations, such as the dynamic region Monte Carlo (DRMC) method [5]. To model the emission or absorption with random numbers accurately requires a weighted sampling as different sections of the spectrum carry different importance. Thus, Importance Sampling comes into the problem where non-uniformly distributed data are to be sampled. The objective of this sampling method is thus to reduce the estimation variance of Monte Carlo estimators without increasing the number of packets or rays to be tracked. Feldick and Modest [6] introduced a variance reduction methodology by implementing the importance sampling to sample wavelengths in the MCRT algorithm.

A better replacement to uniform random numbers is using deterministic, quasi-random sequences. They possess better

space-filling performance than the uniform random number generator and give rise to a low variance, stable Quasi-Monte Carlo (QMC) estimators with faster convergence. Various low-discrepancy sequences are introduced, namely, the Halton [7], Sobol [8] and Faure [9] sequences. Kersch *et al.* [10] demonstrate the improvement in computation time through the introduction of the quasi-random sequences instead of the uniform random numbers to the PMC method. Recently, significant contributions have been made into this method. Palluotto *et al.* [11] used the Halton sequence to develop a randomized QMC to address Radiative transfer problems with 3D participating media. Farmer [12] presented a detailed analysis of QMC for combustion process. Farmer and Roy [13] investigated the computation time benefits with QMC as compared to the standard PMC method with the help of the Sobol sequence. Also, in a different work [14] they presented a comparison using Niederreiter sequence in addition to the other two as well.

In this paper, the effect of Halton, Sobol and Faure sequences is studied for the radiative transfer. The effects of emission and absorption are included along with the influence of participating media in a 1D medium-surface radiation exchange problem. A QMC method is developed, and comparison of results with the line-by-line (LBL) method is presented in the context of computation time, variance, and accuracy. The participating media is taken to be CO (4+) and the spectrum data of absorption coefficient (κ_λ) is modeled with an importance sampling approach such that normalized κ_λ values can be used in the Monte Carlo simulations.

2. METHODOLOGY

For many applications such as combustion, shock waves, hypersonic flow, etc. the emission and absorption from CO (4+) band system are of significant importance. The CO (4+) spectrum is shown in figure 1.

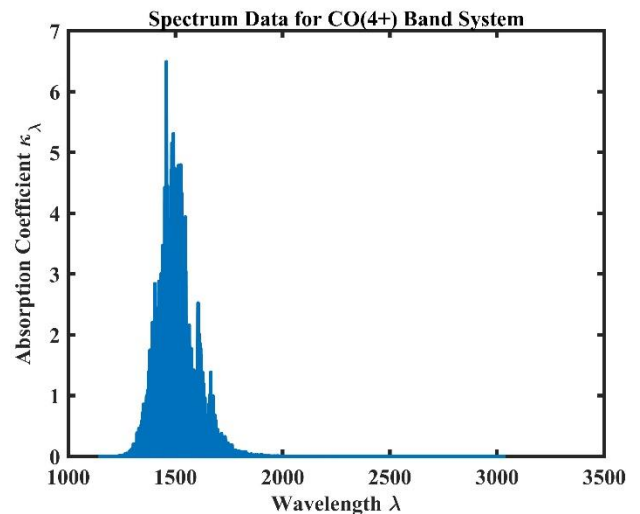


Figure 1: SPECTRUM OF CO (4+) BAND SYSTEM

The first objective of this work is to implement an importance sampling method to perform effective sampling of the spectrum data for the PMC method in non-grey media. Importance Sampling (IS) of wavelengths is based on the importance of a wavelength in its contribution to the calculation of overall heat transfer. The effectiveness of using such a method is well presented for hypersonic flow radiation problems in [6].

It is very important to obtain the values of the absorption coefficient (κ_λ) wisely. Uniform sampling may choose values of κ_λ , which will either result to absorption of the ray before hitting the surface or attenuation to a negligible energy when reaching surface. In order to achieve effective sampling, the proposal function considered was the blackbody spectral intensity itself i.e.

$$I_{b\lambda}(\lambda, s) = \frac{2\pi h c_0^2}{\pi n^2 \lambda^5 [e^{\frac{hc_0}{n\lambda kT(s)}} - 1]} \quad (2)$$

where s is the path coordinate and $I_{b\lambda}$ is the Planck blackbody function. This denotes the intensity possessed by the ray at wavelength λ and position s . If only the intensity is treated as the importance of the wavelength, it would be quite misleading as even wavelengths with high absorption coefficient will be present in high numbers. In such cases even a high energy photon bundle will get absorbed and will not contribute to the energy transferred. So, the importance weights should also include the absorption coefficient directly. And more weight should be given to (λ, κ) pairs that demonstrate higher energy as well as smaller attenuation factor. Hence, the importance weights were calculated as

$$w_\lambda = \frac{I_{b\lambda}}{\kappa_\lambda} \quad (3)$$

where w_λ is the importance given to wavelength λ from the spectrum data. Finally, the spectrum data were sampled to give the updated X_i 's according to the Roulette Wheel Method for the obtained weights. After this step, the Monte Carlo algorithm was implemented.

For a one-dimensional radiative heat transfer problem in medium-surface exchange, two infinite parallel plates were considered with the CO (4+) participating media present in between them as shown in figure 2. The plates are considered to be black and maintained at 0 K. Thus there is no reflection and emission phenomena taking place at the plates. The temperature distribution throughout the media is known and is denoted as $T(x, y)$. A limited number of packets (N) were emitted from the media and tracked throughout the simulation process, and the net heat flux was calculated.

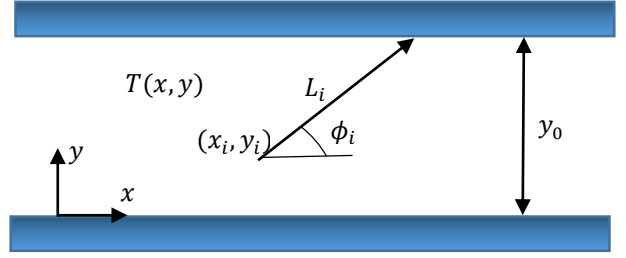


Figure 2: PARALLEL PLATE MEDIUM-SURFACE RADIATION EXCHANGE

The plate at $y = y_0$ and medium between the plates at $y = 0$ and $y = y_0$ is referred for further calculations. The position (x_i, y_i) and angle of emission (ϕ) were calculated according to:

$$x_i = R_x \quad (4)$$

$$y_i = R_y \quad (5)$$

$$\phi_i = 2 * \sin^{-1}(R_\phi) \quad (6)$$

where R_x , R_y , R_ϕ are random numbers and $i = 1$ to N . The values of λ and κ_λ were obtained from the importance sampling results and the attenuation criterion used was related to calculation of the length factor (l_k) as:

$$l_k = \frac{1}{\kappa_\lambda} \log(R_\lambda) \quad (7)$$

where R_λ is a randomly generated number. The photon was considered absorbed if the total distance that has to be traversed by the photon to hit the next surface, L_i (shown in figure 2) is greater than this length factor l_k .

Let us assume radiative transport along a given path with a gray absorption coefficient and known temperature variation. Assuming no wall emission (or cold walls), the intensity of radiation (I_λ), coming out of the media along the path, can be written as in equation (2). The total energy (E_{total}) that is transferred from the medium to the surface of the plate at $y = y_0$ is calculated as the summation of energy carried by rays for all the values in spectrum data. Thus,

$$E_{total} = \int_0^\infty \kappa_\lambda I_{b\lambda} d\lambda \quad (8)$$

Numerically, equation (8) can be written as

$$E_{total} = \left(\sum \kappa_{\lambda_i} I_{b\lambda_i} \right) d\lambda \quad (9)$$

$$d\lambda = \frac{\lambda_{max} - \lambda_{min}}{N_{data}} \quad (10)$$

where summation is done for all the λ values and N_{data} is the number of wavelengths given in the spectrum data. This total energy is divided into the N photon bundles, the wavelength and absorption coefficient values for which were determined through importance sampling. The number of bundles hitting the surface was recorded and hence the net energy transferred from the medium to the surface was calculated.

To model non-gray radiative transport along a path with the Quasi PMC method, the same importance sampled data was used for the values of λ and κ_λ . Let us consider the number of random variables for the Monte Carlo simulation, the Halton, Sobol and Faure sequences are chosen to be 4-dimensional in nature. Each of the dimension will be used for the random numbers responsible for deciding the coordinate of emission (x_i 's and y_i 's), the angle of emission (ϕ) and the length factor (l_k), namely R_x, R_y, R_ϕ and R_λ .

The Halton set is generated as a set of d-dimensional points [15], where each element of a dimension is a point in the Halton sequence. More specifically, the sequence uses the sum of the primes, p , each multiplied with a coefficient given by the base p digits of the non-negative numbers less than p . Such a sequence results in more uniformity than the random generators. Although the random generators also achieve uniformity but with a large number of samples as compared to the low-discrepancy sequence. The star discrepancy of such a sequence can be shown to be of the complexity $O(n^{-1}(\log n)^5)$. The Sobol set was generated similarly using the algorithm [16] considering the direction numbers and bitwise exclusive-or operator. This sequence offers a lower discrepancy resulting in faster convergence and more stable estimates. A major difference in performance is expected because of the change in the space-filling performance of such low-discrepancy sequences as compared to the uniform random number generator.

3. RESULTS AND DISCUSSION

This section compares the results and the computation time using the PMC with and without IS, and the QMC method. The 1D problem was constructed as in figure 2. The temperature distribution $T(x, y)$ throughout the participating media is taken to be constant in x, y for simplicity, given as,

$$T(x, y) = 6000 \text{ K},$$

And the considered plate is taken at a y_0 value of 1 meters. After defining the problem, the PMC algorithm was implemented in the environment. Let the number of photon packets emitted be N . For each packet, the ray was traced and the length of the path was determined. The attenuation factor (l_k) was calculated. Comparing l_k with the length of the ray, it was validated if the ray was able to hit the surface. Once the validation is successful, the photon bundle is believed to fully transfer its energy to the surface. The spectrum data was importance sampled through the

importance weights as in equation (3) to get the sampled wavelengths. The values of κ_λ with respect to each wavelength (λ) were also calculated from the spectrum data of CO (4+) band system. Thus, all the required values are collected and the intensity transferred through the energy packet is calculated. Finally, the process was repeated for all the N rays and the net energy transferred is obtained.

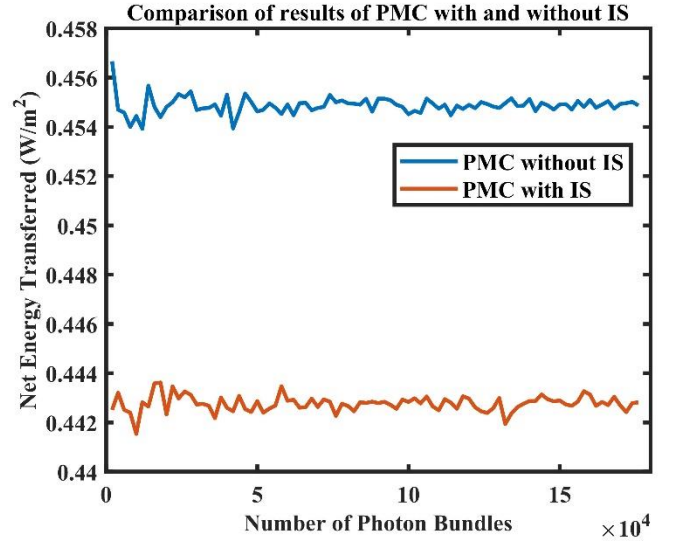


Figure 4: COMPARISON OF RESULTS BETWEEN PMC WITHOUT IS AND WITH IS
(NOTE THAT THE LOWER END OF THE VERTICAL AXIS IS NOT ZERO)

The absolute difference in the values to which the algorithm converges with and without Importance Sampling (IS) is nearly 1.8 %. The difference cannot be considered significant. With the application of IS there is a variance reduction from 1.2×10^{-7} to 1.04×10^{-7} , even for such a simple 1D problem. Thus the variance obtained was less for the Importance sampling based method than the traditional PMC. This shows the effectiveness of the method, although the figure shows various approximations by the Monte Carlo methods for different number of packets.

For the QMC method, the uniform random numbers for the emission coordinate, emission angle and attenuation coefficient was replaced with the Halton sequences and the process was repeated for various values of N . Similar process was conducted with Sobol and Faure numbers and the net energy transferred is compared with each case for same values of N as well as various values of N from 2000 to 200000, as shown in figure 5.

It can be observed that at low number of packets, the variance is quite large for all the 4 methods, more for PMC with uniform random numbers. Although, with the increase in number of packets, as it can be seen in figure, the absolute variance is minimized for the case of QMC with pseudo random numbers. Also, the time elapsed is far more less than the general PMC for the same number of packets as depicted by the figure 6.

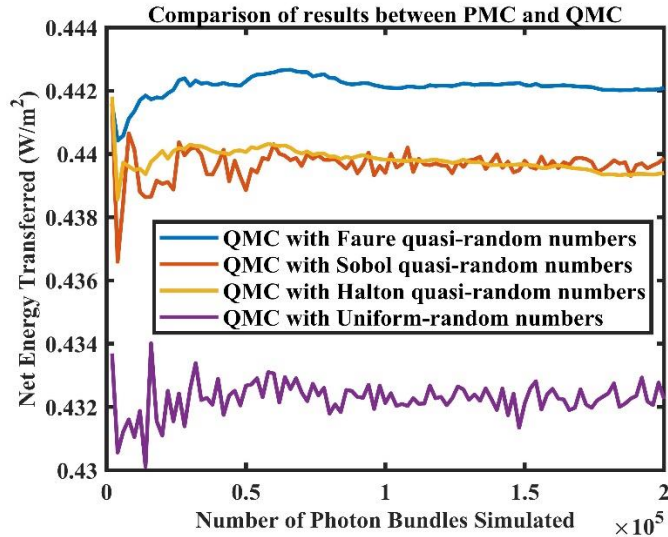


Figure 5: COMPARISON OF RESULTS BETWEEN PMC WITH UNIFORM RANDOM NUMBERS, QMC WITH HALTON, SOBOL AND FAURE QUASI-RANDOM NUMBERS
(NOTE THAT THE LOWER END OF THE VERTICAL AXIS IS NOT ZERO)

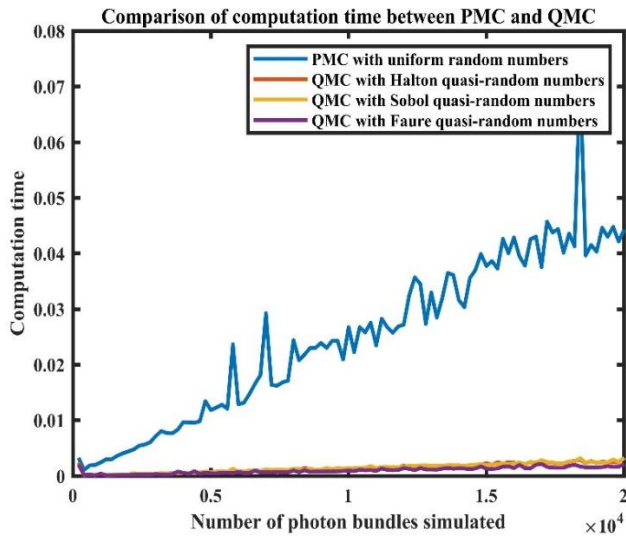


Figure 6: COMPARISON OF COMPUTATION TIME (IN SECONDS) BETWEEN PMC WITH UNIFORM RANDOM NUMBERS, QMC WITH HALTON, SOBOL AND FAURE QUASI-RANDOM NUMBERS

This shows that the sequence perfectly suits the random space filling criterion for this case. Although, other low discrepancy sequences like Niederreiter sequence are expected to give better results.

Hence, importance sampling is used to decrease the variance and quasi-random number sequences are used to decrease the computation time. Thus, an overall reduction in variance and computation time is achieved by the method presented.

Although, none of the methods compared so far are wrong or less correct than others.

4. CONCLUSION

The study addresses an old problem of one dimensional surface-surface radiative heat exchange phenomenon, with modern random number schemes. Photon Monte Carlo (PMC) has been a topic of interest since the last 2 decades due to its capacity of accurately solving the RTE with all the emission, absorption, scattering and participating media effects. Recently, the introduction of the use of various low discrepancy sequence has opened up various extensions to the PMC method. The Quasi Monte Carlo (QMC) scheme, as established through the study, is equally accurate (within 2% of the general PMC results) to the PMC scheme but has the advantage of low variance and less computation time over it.

Also, various low discrepancy sequences with their order of star discrepancy, provide different space filling sequences and hence different results with QMC. Pseudo Random Number generation through randomized Halton points proved to be both fast in time and more successful in variance reduction. On the other hand, Sobol sequence proved to have a higher rate of convergence than the simplest Halton points scheme, having a lower order of the star discrepancy. In addition to all these, the addition of Importance Sampling (IS) played a vital. IS helps in decreasing the variance obtained with uniformly generated random numbers for the same value of N .

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