Proceedings of the 9th International Symposium on Radiative Transfer, RAD-19
June 3–7, 2019, Athens, Greece

RAD-19-CS01

A PHOTON MONTE CARLO SOLVER UTILIZING A LOW DISCREPANCY SEQUENCE FOR THERMAL RADIATION IN COMBUSTION SYSTEMS

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ABSTRACT. Monte Carlo-based radiation solvers can provide an accurate solution to thermal radiation transfer in nongray participating media. Unfortunately, the computational cost of Monte Carlo solvers is an impediment to their use in large-scale simulations. A deterministic sampling-based quasi-Monte Carlo (QMC) method is proposed in this work as an efficient alternative to conventional Monte Carlo solvers. This QMC uses a low discrepancy sequence instead of random sampling required in Monte Carlo-based approaches. The implementation is validated in one-dimensional configurations and is further tested in three-dimensional nonhomogeneous configurations. QMC shows generally better error convergence rates. In three-dimensional cases QMC produces a similar level of error compared to a conventional Monte Carlo solver without having to run multiple statistical instances. This leads to significant computational cost benefits from QMC as seen in the Figure of Merit comparison between QMC and conventional Monte Carlo.

1. INTRODUCTION

Thermal radiation can play a significant role in heat transfer especially in combustion applications. Several researchers have pointed out the importance of accurate radiative solution for combustion systems [e.g., see 1, and references therein]. Radiative heat transfer in participating media is governed by the spectral radiative transfer equation (RTE) [2]. The RTE, which is shown in Eqn. 1, is a five-dimensional integro-differential equation for radiative intensity and includes influence from emission, absorption, and scattering.

$$\frac{dI_\eta}{ds} = \hat{s} \cdot \nabla I_\eta = \kappa_\eta I_{b\eta} - \beta_\eta I_\eta + \frac{\sigma_{s\eta}}{4\pi} \int_{4\pi} I_\eta(\hat{s}) \Phi_\eta(\hat{s}_i, \hat{s}) d\Omega_i, \tag{1}$$

where the subscript η denotes the equation is valid for one single wavenumber η. Here I stands for radiative intensity, I_b is blackbody radiative intensity, κ is absorptivity of the medium, β is extinction coefficient, σ_s is scattering coefficient, $\Phi(\hat{s}_i, \hat{s})$ is the scattering phase function between ray directions $\hat{s}_i$ and $\hat{s}$, and Ω_i represents solid angle. Radiative properties of the medium (κ, σ, β and Φ) vary with wavenumber and thermodynamic states in a highly nonlinear manner. This makes direct solution of the RTE over all spectral wavenumbers a complex problem.

The available solution methodologies for the RTE can be categorized as deterministic and stochastic. Deterministic RTE solvers essentially transform the integro-differential equation into a set of partial differential equations (PDEs) by performing a variety of discretization [see e.g., 2,3, etc.]. The stochastic approach to RTE has lead to a series of Monte Carlo based solvers. All of which essentially solves the radiative transfer process by tracing a large number of photon bundles or rays. This category of solvers are often referred as photon Monte Carlo (PMC) solvers [4]. With sufficiently

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large number of rays these solvers can reproduce the exact solution to the RTE. The main advantage of PMC solvers are their accuracy, apparent simplicity, and robustness. The complexity of the solver is not affected by presence of scattering or reflection, or complex geometry. However, the main bottleneck is the computational cost. For an accurate PMC solution, these methods require multiple statistical analyses over a very large number of rays. Therefore, although PMC can produce the exact solution to the radiation transfer problem, it is impractical to use in routine large-scale simulations.

This work presents a detailed validation study of an efficient alternative to PMC solvers by using low-discrepancy sequences (LDS). This approach leads to a quasi-Monte Carlo (QMC) solver for radiation. It is shown in the current study that QMC can lead to same level of accuracy at a fraction of cost of PMC both in simple one-dimensional canonical configuration as well as in three-dimensional configurations.

2. MONTE CARLO-BASED RTE SOLVERS

2.1 Standard Monte Carlo Ray Tracing

The Monte Carlo (MC) ray tracing or photon Monte Carlo (PMC) method accounts for radiative transfer by mimicking the process of energy transfer via electromagnetic radiation by emitting and tracing a large number of rays or photon bundles. Each ray has a finite amount of energy and as it passes through the participating medium, the medium absorbs some of its energy according to the radiative properties of the medium. Each ray (denoted by index j) is defined by the origin (x_j, y_j, z_j), propagation direction (θ_j, ϕ_j), wavenumber (η_j) and initial energy content (E_j^o). The first six parameters are obtained by sampling six independent, uniformly distributed random numbers ($R_x, R_y, R_z, R_\theta, R_\phi$, and R_η). Initial energy of the ray is calculated from total energy of the origin location and number of rays emitted from the location as $E_j^0 = {}^{E_i}/_{N_i}$, where E_i is the energy of the computational cell i which contains the location of origin of the ray, and N_i is the number of rays emitted from cell i. The details of these processes are discussed in detail in the literature [e.g. 2,4–7, etc.].

Typically, the accuracy of Monte Carlo (MC) methods are estimated by the statistical error – the standard deviation of an evaluated variable over multiple statistical iterations. Theoretically, the error limit of Monte Carlo methods with N samples (in this case, N rays), is represented by $O(N^{-0.5})$. The computational cost of MC methods, on the other hand, usually increases linearly with the number of samples. Therefore, the rate of increase of computational cost supersedes the rate of decrease of standard deviation. This has been a serious bottleneck for PMC to be useful in large-scale simulations. Therefore the use of PMC is commonly restricted as a benchmark RTE solver and validation tool in complex radiative heat transfer problems. In this document we use the abbreviation MC and PMC interchangeably to represent the standard Monte Carlo-based RTE solver.

2.2 Quasi-Monte Carlo

The term *quasi-Monte Carlo* refers to MC methods that use quasi-random sampling in lieu of true random or pseudorandom sampling [8]. A good random number generating algorithm is deceptively complex. Often in numerical applications a pseudorandom generator is used to generate random samples. Pseudorandom numbers are not truly stochastic; they are generated using a deterministic algorithms, but still satisfy the statistical properties of a uniform random distribution reasonably well [9]. To increase robustness, the pseudorandom numbers are sometime used with a true-random seed harvested from physical environment, such as a time counter or thermal noise. Quasi-Monte Carlo, on the other hand, does not use a random sampling at all. Instead, it uses a low-discrepancy sequence (LDS) to generate samples [8]. A low-discrepancy sequence is multidimensional sequence

designed to reduce variance.

An LDS has an advantage over random/pseudorandom numbers in that it "covers" the entire domain quickly and more evenly. Although these sequences share properties with pseudorandom numbers, an LDS is a deterministic routine specifically designed to have equidistant points in a plane. The use of LDS in Monte Carlo-based solvers have been in development for many years [8]. Such applications have shown great promise in other fields such as financial modeling [10], computer graphics [11], etc. QMC has shown preliminary success in simple RTE problems [12,13]. More recently, a QMC-based approach has also been used in the context of combustion simulation [14].

In this work, Sobol's sequence was chosen as the target LDS based on empirical study of the computational expense and the recommendations of [15,16]. In the QMC using Sobol's sequence, a six-dimensional Sobol sequence is used to replace the six random numbers from the standard PMC method. So $R_x, R_y, R_z, R_\theta, R_\phi, R_\eta$ required to define ray j in MC are replaced with $S_j^1, S_j^2, \ldots, S_j^6$ in QMC, where S_j^n indicates j^{th} number in n^{th} dimension of the Sobol sequence. In case of rays emitted from wall surface, the dimensionality of the problem is reduced as ray origin on a wall face can be identified by only two coordinates. For such cases we simply ignore the corresponding S_j^3. Further investigations are needed if this may affect efficiency of QMC. It is noted here, that to in presence of scattering and reflective surfaces, more than six random numbers are needed in MC and therefore additional dimensions of LDS need to be investigated. This study, however, does not include scattering and reflection, which are left for future work. For more details on LDS, Sobol's sequence, and QMC the reader is directed to respective literature [e.g. 8,17,18, etc.].

3. RESULTS

3.1 Target configurations

In this work, we propose an implementation of QMC as an efficient alternative to MC (aka PMC). To that end, we first present validation of QMC in a one-dimensional configuration where an analytical solution is available, followed by a performance comparison of MC and QMC in a couple of three-dimensional configurations relevant to combustion. It is noted here that several gray and nongray one-dimensional cases were used for validation but only one representative configuration is shown here for brevity. All configurations presented here contains nongray media, and CO_2, H_2O, and CO are treated as the participating species. The spectral radiative properties are obtained using a line-by-line (LBL) database constructed from the HITEMP spectroscopic database [19]. The target variables that are compared are local divergence of the radiative heat flux ($\nabla \cdot Q$) or local radiative absorption as suited for each case.

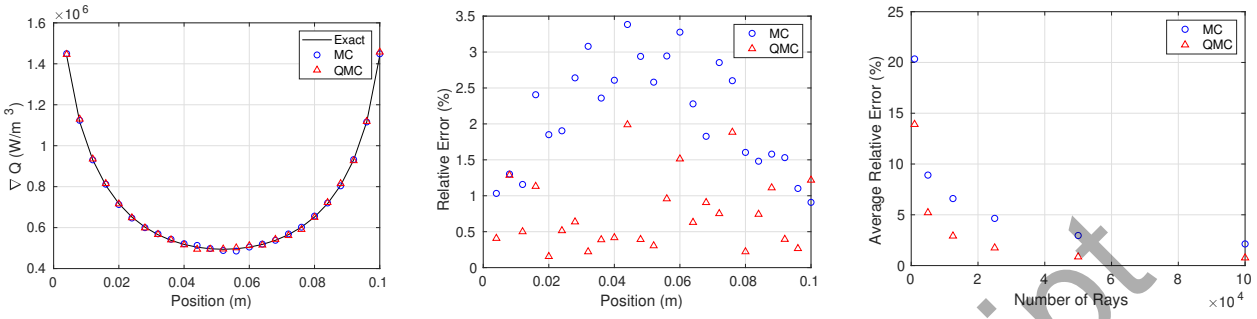
For both MC and QMC, the accuracy of each method is shown in terms of the root mean square (RMS) relative error at each computational cell i and the variation of averaged RMS relative error with number of rays used in each simulation. The RMS relative error at computational cell i is defined by

$$\epsilon_i = \left(\frac{1}{S} \sum_{s=1}^{S} (q_i^s / q_i^o - 1)^2 \right)^{1/2}, \tag{2}$$

where S is the number of statistical runs, q_i^s is the simulation result from one run, and q_i^o is the exact/benchmark solution at the cell i. For Monte Carlo simulations $S = 10$ statistical runs were performed. Since QMC uses a deterministic sequence, and two independent runs will always generate same sequence, only one run is required for QMC. Average RMS relative error $\bar{\epsilon}$ is calculated as spatial average of local RMS relative error ϵ_i.

3.2 One-Dimensional Plane-parallel Medium

For the one-dimensional case, a nonscattering, nongray, gaseous, plane parallel medium, with cold (non-emitting) and black walls is used. The temperature of the medium is uniform at 2000 K, the distance between the walls are 0.1 m, and the medium was composed of H_2O with a mole fraction of 0.25.



(a) Comparison of $\nabla \cdot Q$ for simulations with 100,000 rays

(b) Local RMS relative error (ϵ_i) for simulations with 100,000 rays

(c) Decrease in average error ($\bar{\epsilon}$) with number of rays

Figure 1. Accuracy and convergence rates for 1D case

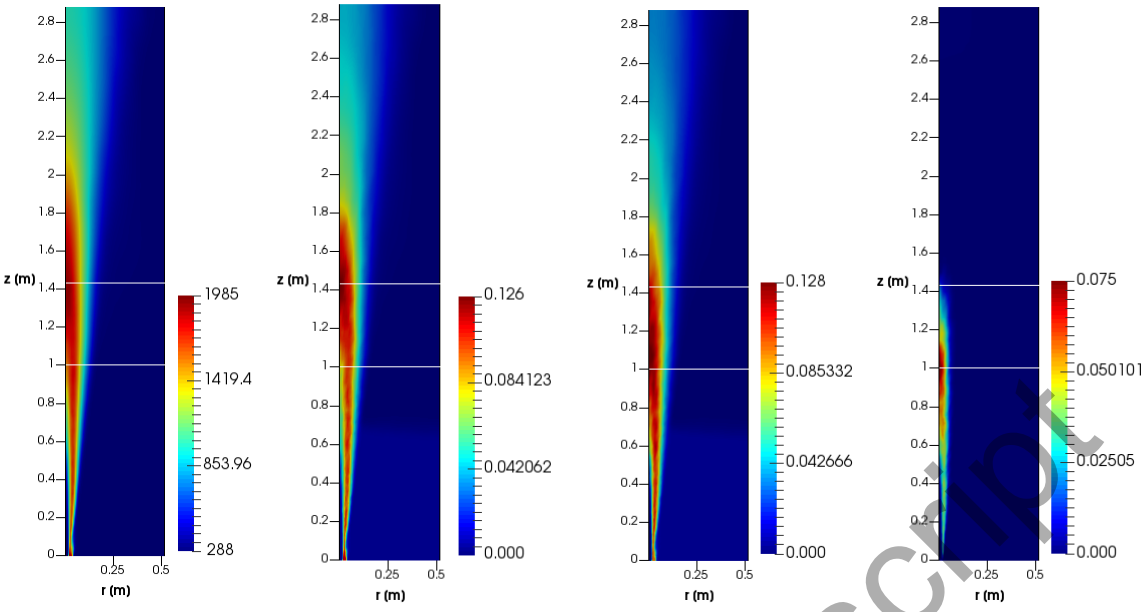
Figure 1 presents the results for the MC, and QMC methods. Both methods show excellent agreement with the analytical solution as seen in Fig 1(a). Figure 1(b) demonstrates the variation of RMS relative error (ϵ_i) with location and it can be seen that error from QMC is generally lower than that from MC. Figure 1(c) shows the 'convergence rate' of the solvers. The convergence rate is defined as the rate at which the averaged RMS relative error ($\bar{\epsilon}$) decreases with number of rays used in a simulation. These figures show that the performance of QMC is better than MC in terms of accuracy for any given number of rays. A point to note here, the errors are obtained from only one run of QMC with N rays and $S = 10$ statistical runs of MC with N rays. This alludes to the fact, that QMC can achieve significant accuracy vs. cost advantage of MC in one-dimensional configuration.

3.3 Combustion-Relevant Simulations

Two combustion-relevant cases are considered here. The first case is a snapshot of scalar fields from an artificial flame based on the turbulent nonpremixed Sandia-D flame [20]. This flame was artificially scaled up by quadrupling the dimensions and reducing the velocities appropriately to maintain the same Reynolds number [21,22]. A snapshot of the scalar field of this flame is shown in Fig. 2 and is referred as SandiaDx4 configuration. This configuration has 3,325 computational cells. The second configuration is based on the combustion chamber of an industrial gas turbine with approximately 5 MW output and a pressure ratio of approximately 15:1 [23]. A snapshot taken from the numerical simulation of this gas turbine by Ren et al [24] is shown in Fig. 3. This configuration is referred as GT configuration and has 15,718 computational cells with five, black walls emitting at 673 K. Effect of wall emission and reflection on the uniformity of LDS in thermal radiation will be the topic of future discussions. Although the configurations are axisymmetric, the actual simulations are done in three-dimensional meshes. Both the flow/combustion solver (OpenFOAM, in this case) and the Monte Carlo solver solve full three-dimensional set of equations.

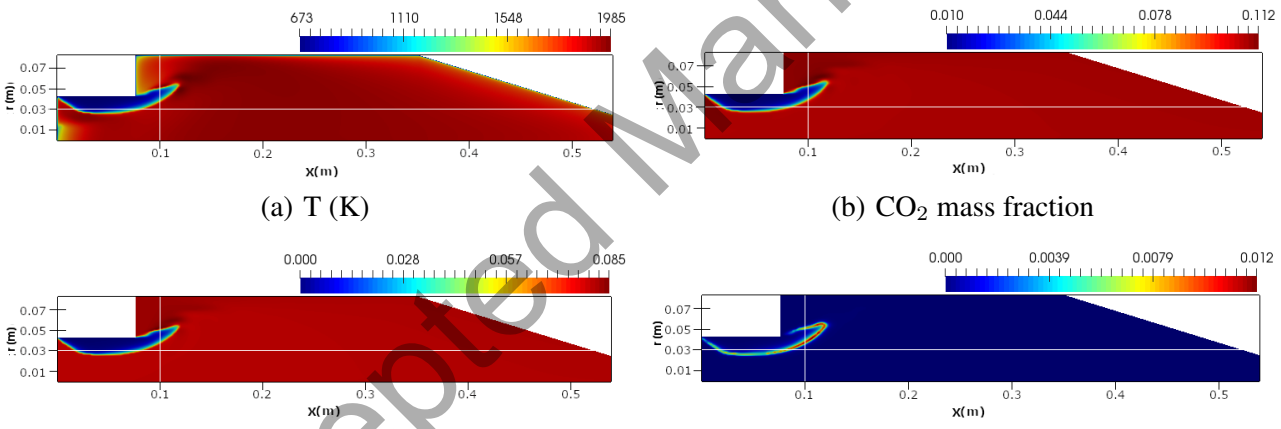
Unlike one-dimensional configurations, an analytical solution is impossible to obtain for three-dimensional non-homogeneous non-gray media. Solutions calculated from 50 statistical runs of a MC simulation with 5×10^6 rays for the SandiaDx4 configuration and 10^7 rays for the gas turbine (GT) configuration are treated as the benchmark solutions for the purpose of evaluating RMS error as shown in Eqn. 2. It should be noted here that the benchmark solution is not expected to be "exactly" the correct solution but instead thought of as "close enough," and probably favors the MC method in

terms of relative error, anyway.



(a) T (K) (b) CO_2 mass fraction (c) H_2O mass fraction (d) CO mass fraction

Figure 2. Scalar field contours for SandiaDx4 configuration



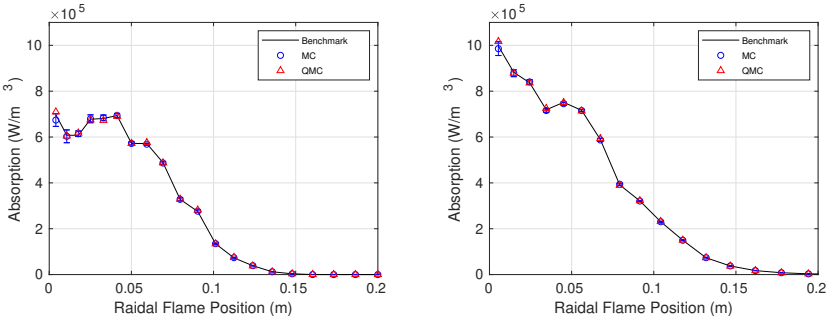
(a) T (K) (b) CO_2 mass fraction

(c) H_2O mass fraction (d) CO mass fraction

Figure 3. Scalar field contours for GT configuration

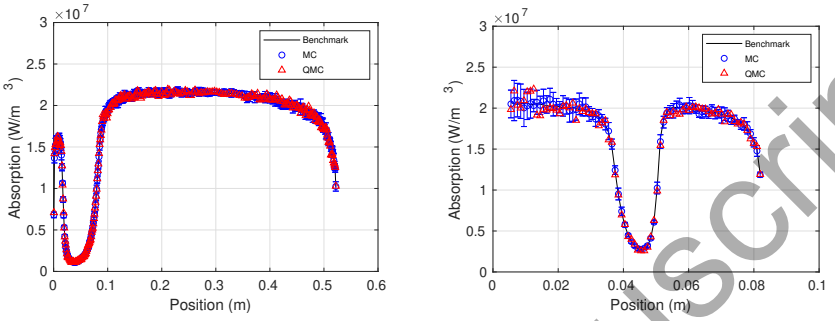
Instead of the divergence of radiative heat flux the comparison of different solvers are made in terms of absorption in these cases. This choice is made because of the presence of locally strong optically thick regions. Optically thick regions will show strong emission and absorption leading to a near-zero value of $\nabla \cdot Q$. Therefore calculation of relative error based on $\nabla \cdot Q$ can be misleading. Moreover, local emission can be determined completely based on Planck-mean absorption coefficient and temperature and the uncertainty of the radiative transfer in MC/QMC comes from the randomness in resolving the absorption term.

Figure 4 shows radial profiles of absorption at two different axial locations of the SandiaDx4 configuration. The axial locations are marked in Fig. 2 at, respectively, z = 1.0 m, and 1.43 m where the results were taken. Figure 5 shows similar radial and axial profiles for the GT configurations and Fig. 3 show the marked axial profile at r = 0.03 m and radial profile at x = 0.1 m locations. In both Figs. 4 and 5 an error bar based on one standard deviation is added to the MC results. It is evident from Fig. 4 and 5 that results from QMC agrees well with the benchmark solution and within one standard deviation of corresponding MC result.



(a) Radial profile along 1.0 m (b) Radial profile along 1.43 m

Figure 4. Absorption along a line in SandiaDx4 configuration with 800,000 rays



(a) Radial profile along 0.03 m (b) Axial profile along 0.1 m

Figure 5. Absorption along a line in GT configuration with 1,600,000 rays

As discussed earlier, one key advantage of QMC is its deterministic sampling requires only one statistical run to estimate error. This can lead to significant computational savings. To quantify this, a "figure of merit" (FoM) can be used to evaluate and compare the performance of a Monte Carlo simulation [4]. FoM can be defined as

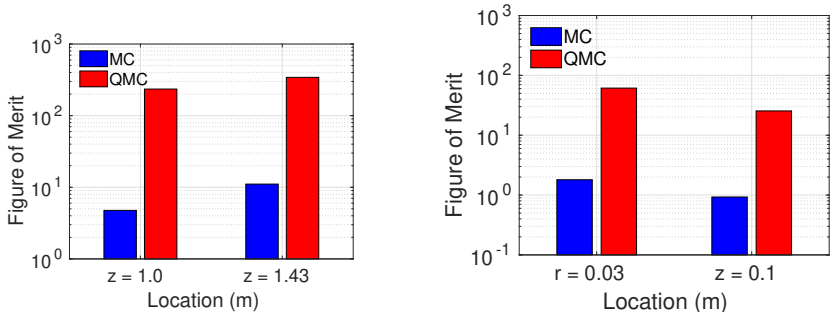
$$\text{FoM} = \frac{1}{\bar{\epsilon}^2 t}, \tag{3}$$

where t is the computational time. In this work, FoM is calculated based on spatially-averaged RMS relative error ($\bar{\epsilon}$). A high FoM score indicates low error at low computational cost, i.e., a good Monte Carlo simulation. Figure 6 shows the FoM along a line for each line marked in Figs. 2 and 3 for SandiaDx4 and GT, respectively. Figure 6 shows consistent positive results in each case for QMC. This can be attributed to the fact that for a given number of rays, QMC and MC have similar level of accuracy but MC simulations require several statistical runs while the QMC needs to run only once due to deterministic sampling, effectively creating an order of magnitude difference in FoM. It is noted here that between one single MC run and a QMC run there is no significant computational cost difference.

Figure 7 shows how the FoM varies with number of rays for both QMC and MC simulations. For MC simulations it is found that the FoM remains almost constant as the number of rays is increased. This outcome is expected due to the statistical error limit being $O(N^{-1/2})$ and computational cost of ray tracing being approximately proportional to number of rays, N. Interestingly, QMC also shows similar trends in these cases. Further investigations of this is left for future.

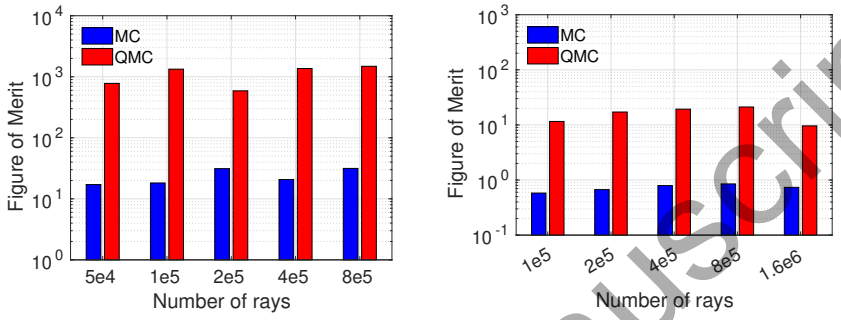
4. CONCLUSION

Monte Carlo-based radiation solvers are accurate, robust, but computationally costly. In this work an implementation of quasi-Monte Carlo using a low-discrepancy Sobol's sequence was validated and



(a) SandiaDx4 with 800,000 rays (b) GT with 1,600,000 rays

Figure 6. Figure of Merit (FoM) along two different lines of MC and QMC simulations for SandiaDx4 and GT configurations.



(a) SandiaDx4 profile at z=1.43 m (b) GT profile at r=0.03 m

Figure 7. Figure of Merit (FoM) with change in number of rays

tested first in canonical one-dimensional configuration and then in combustion-relevant configurations. QMC shows similar and often lower level of error than MC in the cases studied. Because of the deterministic sampling, QMC also eliminates the requirement of statistically significant number of MC simulations to obtain an error estimate. The combined effect of this can be clearly seen in significantly higher Figure of Merit of QMC solver than MC solver particularly in combustion simulations. This preliminary study shows clear benefits of QMC. Further investigations on advantages and limitations of QMC in different combustion configurations are being left for future.

ACKNOWLEDGMENTS

This material is based upon work supported by the National Science Foundation (NSF) under Grant No. 1756005.

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