A Quasi–Monte Carlo Method With Krylov Linear Solvers for Multigroup Neutron Transport Simulations

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Abstract — In this work we investigate replacing standard quadrature techniques used in deterministic linear solvers with a fixed-seed Quasi–Monte Carlo (QMC) calculation to obtain more accurate and efficient solutions to the neutron transport equation (NTE). QMC is the use of low-discrepancy sequences to sample the phase-space in place of pseudorandom number generators used by traditional Monte Carlo (MC). QMC techniques decrease the variance in the stochastic transport sweep and therefore increase the accuracy of the iterative method. Historically, QMC has largely been ignored by the particle transport community because it breaks the Markovian assumption needed to model scattering in analog MC particle simulations. However, by using iterative methods the NTE can be modeled as a pure-absorption problem. This removes the need to explicitly model particle scattering and provides an application well suited for QMC. To obtain solutions we experimented with three separate iterative solvers: the standard Source Iteration (SI) Solver and two linear Krylov Solvers, i.e., the Generalized Minimal RESidual method (GMRES) and the BiConjugate Gradient STABilized method (BiCGSTAB). The resulting hybrid iterative-QMC solver was assessed on three slab geometry problems of one dimension. In each sample problem the Krylov Solvers achieve convergence with far fewer iterations (up to eight times) than the SI Solver. Regardless of the linear solver used, the hybrid method achieved an approximate convergence rate of \(O(N^{-1})\) as compared to the expected \(O(N^{-1/2})\) of traditional MC simulation across all test problems.

Keywords — Neutron transport, Monte Carlo methods, Quasi–Monte Carlo, Krylov linear Solvers.

Note — Some figures may be in color only in the electronic version.

I. INTRODUCTION

Solving the neutron transport equation (NTE) accurately and efficiently under various conditions is vital to nuclear reaction simulations like those in advanced reactor design or accident analysis.1 The NTE describes the distribution of neutrons in space, angle, energy, and time. The equation’s high-dimensional nature makes it difficult to design efficient general-purpose algorithms, and many solution techniques, most common of which have been stochastic Monte Carlo (MC) simulations2 or deterministic discrete ordinates \(S_n\) methods,3 have been developed.

For deterministic solutions, Source Iteration (SI) is the simplest and most common deterministic solution technique for solving the discrete ordinates method.5 SI is equivalent to a fixed-point Picard iteration and as problems become collision dominated, the convergence rate of the SI can become arbitrarily slow.4,5 More advanced iteration techniques such as Krylov subspace methods, including the Generalized Minimal RESidual method (GMRES) and the BiConjugate Gradient STABilized method (BiCGSTAB), have been shown to outperform standard SI, particularly when there are highly scattering materials.4 Nonetheless, as the dimensionality and fidelity of the problem increase, the deterministic quadrature techniques used to evaluate the system of equations become intractable.6,7
Monte Carlo simulations provide a more robust solution by using random sampling and probability to produce solutions. In this method the statistical error scales according to $O(N^{-1/2})$, where $N$ is the number of neutron histories—regardless of the dimensionality of the problem. However, MC simulations are often seen as a last resort because of their high computational cost and slow rates of convergence. Recent work by Willert\textsuperscript{7} and Willert et al.\textsuperscript{12} investigated a hybrid MC-deterministic solution where the deterministic quadrature sweep of the iterative method was replaced with a MC transport simulation. This method attempts to combine the efficiency of iterative methods while also providing an accurate solution for complex problems given the robustness of MC simulation. However, it is found that a staggering number of particle histories may be required for convergence of the iterative method even for monoenergetic slab problems.\textsuperscript{12} Or, as Von Kleist wrote in a previous age, \textsuperscript{13} “probability is not always on the side of truth.”

Our work investigates the use of fixed-seed Quasi-Monte Carlo (QMC) techniques in place of standard, pseudorandom MC to decrease the variance in the transport process and therefore improve the convergence of the iterative method. QMC techniques use low-discrepancy sequences (LDSs) in place of typical pseudorandom number generators for MC sampling. Various LDSs have been developed, including the Sobol and Halton Sequences, and the goal of each is to sample the phase-space in a deterministic and self-avoiding manner. Theoretically, this results in a sampling convergence rate proportional to $O(N^{-1})$ compared to $O(N^{-1/2})$ of standard MC (Ref. 14).

Rather than taking subsequent samples from the same LDS at the start of every iteration, the LDS is reset to the beginning of the sequence. This fixed-seed approach allows the iterative method to converge at a much faster rate than if new samples were taken. With typical random number generators, this technique would be avoided to ensure samples are uniformly distributed through the phase-space. However, the low-discrepancy nature of the Sobol Sequence, Halton Sequence, etc., ensures a well-balanced sampling of the phase-space even with a relatively low number of samples.

Despite the benefits offered by QMC, it has largely been ignored by the particle transport community.\textsuperscript{15} There has been some recent work in using QMC for radiative transfer problems without scattering.\textsuperscript{16,17} But to the knowledge of the authors, there has not been any recent work with QMC applied to neutron transport. This is likely because the deterministic nature of the LDS breaks the Markovian assumption needed for the particle random walk when scattering is present. Therefore, QMC must be implemented in applications that are not Markovian processes, or steps must be taken to ensure the Markovian assumption is maintained.

At present, there have been two strategies for implementing QMC in particle transport. The first is known generally as randomized-QMC (RQMC), which includes a host of strategies that attempt to randomize a sequence and still retain the low discrepancy of the samples.\textsuperscript{15,17–19} Depending on the randomization technique, the theoretical convergence rate of $O(N^{-1})$ may be reduced\textsuperscript{20,21} and other randomization techniques may theoretically uphold the $O(N^{-1})$ convergence rate but become computationally expensive to execute.\textsuperscript{21} The second implementation of QMC in particle transport is in problems without scattering, primarily seen in radiative heat transfer problems.\textsuperscript{16,17}

Our proposed iterative-QMC (iQMC) method allows for both: problems that include scattering and the use of unaltered LDSs; i.e., no RQMC method is required. This is achieved by modeling the problem in the QMC simulation as a purely absorbing system where each particle is emitted and traced out of the volume. After this process, or QMC Sweep as it will be referred to from now on, the scattering term is iterated upon using a deterministic linear solver, and the process repeats until a desired tolerance or maximum number of iterations is reached, thereby removing the need for the simulation of a random walk process.\textsuperscript{22}

The outline of this paper is as follows. Section II.A presents a brief overview of the NTE, SI, and Krylov Solvers. Section II.B describes the use of fixed seeding and LDSs to form the QMC transport sweep. Section III provides an overview of the implemented algorithms before analysis, and Sec. IV presents results from three one-dimensional (1D) test problems. The first problem solves for scalar flux in an infinite medium with multi-group data generated from FUDGE (Ref. 23) with a known analytic solution. The second problem, known as Reed’s Problem, is a multimedia problem benchmarked with results from a high-particle-count MC simulation, using the Center for Exascale Monte-Carlo for Neutron Transport’s (CEMeNT’s) Monte-Carlo Dynamic Code (MCDC) (Ref. 24). The third and final problem, provided by Garcia and Siewert, provides angular flux results at the slab edges from a fixed
boundary source with a spatially decaying scattering cross section.\textsuperscript{20} Finally, key findings and future work are discussed in Sec. V.

\section*{II. METHODS}

\subsection*{II.A. Neutron Transport SI and Krylov Methods}

We begin with the one-speed NTE in slab geometry with isotropic scattering\textsuperscript{3}:

\[
\frac{\partial \psi}{\partial x}(x, \mu) + \Sigma_t(x)\psi(x, \mu) = \frac{1}{2} \left[ \Sigma_s(x)\phi(x) + q(x) \right] \tag{1}
\]

and

\[
\phi(x) = \int_{-1}^{1} \psi(x, \mu) d\mu, \text{ for } 0 \leq x \leq \tau . \tag{2}
\]

the boundary conditions are

\[
\psi(0, \mu > 0) = \psi_l(\mu), \quad \psi(\tau, \mu < 0) = \psi_r(\mu), \tag{3}
\]

where

\[
x, \mu = \text{particle position and angle, respectively} \\
\psi = \text{angular flux} \\
\phi = \text{scalar flux} \\
\Sigma_t = \text{total macroscopic cross section} \\
\Sigma_s = \text{scattering macroscopic cross section} \\
q = \text{internal source function}.
\]

\subsection*{II.A.1. Source Iteration}

Transport Eqs. (1) and (2) can be solved iteratively via SI:

\[
\frac{\partial \psi^{(n+1)}}{\partial x}(x, \mu) + \Sigma_t(x)\psi^{(n+1)}(x, \mu) = \frac{1}{2} \left[ \Sigma_s(x)\phi^{(n)}(x) + q(x) \right] \tag{4}
\]

and

\[
\phi^{(n+1)}(x) = \int_{-1}^{1} \psi^{(n+1)}(x, \mu) d\mu , \tag{5}
\]

where superscript \((n)\) indicates the iteration index. The equations can be represented in operator notation as

\[
\phi^{(n+1)} = S[\phi^{(n)}, q, \psi_l, \psi_r] , \tag{6}
\]

where the transport sweep operator \(S\) updates a scalar flux estimate given an internal source \(q\) and boundary sources \(\psi_l\) and \(\psi_r\). In the proposed hybrid method, this transport sweep operation is performed via MC simulation (which is discussed in Sec. II.B).

The SI Eq. (6) can be rewritten as follows:

\[
\phi^{(n+1)} = K[\phi^{(n)}] + f , \tag{7}
\]

where

\[
K[\phi^{(n)}] = S[\phi^{(n)}, 0, 0, 0] \tag{8}
\]

and

\[
f = S[0, q, \psi_l, \psi_r] . \tag{9}
\]

By collecting the scalar flux terms, one can demonstrate that SI is equivalent to the fixed-point Picard iteration of a linear problem:

\[
A\phi = (I - K)\phi = f , \tag{10}
\]

where \(I\) is the identity function. Equation (10) is in a form we can send to linear solvers, particularly those that are more efficient than the fixed-point Picard iteration, such as Krylov methods. Note that we do not need to explicitly form matrix \(A\); we need only to compute the action of \(A\) on \(\phi\), which is accomplished with the QMC Sweep.

\subsection*{II.A.2. Krylov Methods}

An order-\(r\) Krylov subspace is defined with notation from Sec. II.A.1 as\textsuperscript{26}

\[
K_r = \text{span}(\phi, A\phi, A^2\phi, ..., A^{r-1}\phi) . \tag{11}
\]

For each experiment presented in Sec. IV, two Krylov methods, GMRES (Ref. 27) and BiCGSTAB (Ref. 28), were used. GMRES is one of the most common Krylov methods. When solving \(A\tilde{\phi} = \tilde{f}\), GMRES minimizes \(||f - A\tilde{\phi}||_2\) over the \(k\)th Krylov subspace. For every iteration, GMRES stores an additional Krylov vector. For problems that require many iterations, this may lead to memory constraints. BiCGSTAB is a low-storage Krylov method that is memory bounded throughout the
algorithm. However, the memory savings come from information that is thrown out with each iteration, and therefore, BiCGSTAB will generally require more iterations to converge than GMRES. Nonetheless, as we will observe in Sec. IV, both Krylov methods will require far fewer iterations than SI.

II.B. QMC Transport Sweep

II.B.1. Monte Carlo Transport Sweep

Monte Carlo methods for neutron transport seek to simulate the behavior of a statistically significant number of particles from birth to death to gain an approximate behavior of the system. For our 1D simulations, each particle begins with an initial position \( x_1 \), direction \( \mu_1 \), and statistical weight \( w_1 \). In an analog simulation, the particle would then be tracked from collision to collision, tallying quantities of interest as the particle moves. Each time the particle undergoes a scattering collision, a new direction \( \mu \) would be sampled, and the next distance to collision would be calculated. This process would repeat until the particle is either absorbed or exits the volume. However, Eq. (4) is a purely absorbing transport problem with a known source. MC simulation in a purely absorbing system can be enhanced by employing the continuous weight absorption technique (also called implicit capture), which continuously reduces the statistical weight of each particle per length traveled \( s \):

\[
w_{\text{new}} = w_{\text{old}} e^{-\sum_{i} s}.
\]  

(Eq. 12)

Consequently, after emission the particle is traced straight out of the volume reducing the statistical weight according to the distance traveled across each spatial cell, as illustrated by Fig. 1.

We use the track-length tally estimator to compute the spatially averaged scalar flux in the defined mesh. Because the weight is continuously reduced with each step, the tally scoring becomes

\[
\frac{1}{V} \int_{0}^{\Sigma} w_{\text{old}} e^{-\sum_{i} s} ds = \frac{w_{\text{old}}}{V} \left( 1 - e^{-\sum_{i} s} \right).
\]  

(Eq. 13)

This estimate of the scalar flux is then used to compute the scattering source in the next iteration of the solver.

II.B.2. Low-Discrepancy Sequence for QMC

Given the purely absorbing system, Eq. (4), and the use of the continuous weight absorption technique, Eqs. (12) and (13), the only quantities that need to be randomly sampled are the particle initial position \( x_i \) and direction \( \mu_i \). In a standard MC transport sweep, a pseudorandom number generator is used to sample \( x \) and \( \mu \). In a QMC transport sweep, a deterministic low-discrepancy sequence is used instead, of which there are two primary classes: sequences and integration lattices. Integration lattices can be viewed as a multidimensional analog of the trapezoidal rule. Sequences are much more popular in practice, in part because lattices are difficult to extend to infinite sequences.

Sequences like Sobol and Halton use deterministic algorithms to sample the phase-space in successively finer partitions and then reorder the coordinates in each dimension thereby approaching a more uniform distribution and approximating the expectation more efficiently. This results in a theoretical convergence rate of \( O(N^{-1}) \) compared to the \( O(N^{-1/2}) \) from pseudorandomly placed points. In addition to the well-known Sobol and Halton Sequences, Fig. 2 shows the distribution of 256 points in a unit square of a newer LDS known as the Golden Sequence.

In the context of our 1D, steady-state, neutron transport problems, we generate a two-dimensional (2D) Sobol sequence for the desired number of particle histories \( N \):

\[
\begin{bmatrix}
s_{11} & s_{12} & \cdots & s_{1N} \\
 s_{21} & s_{22} & \cdots & s_{2N}
\end{bmatrix},
\]  

(Eq. 14)

where elements \( (s_{ij} \in [0,1]) \) from the first and second rows are, respectively, mapped to particle \( j \) initial position and angle according to
and

\[
\mu_j = 2s_j - 1, \quad (16)
\]

where \( L \) and \( R \) are the slab-edge boundaries.

**II.B.3. Multigroup Vectorization**

Neutron cross sections vary greatly with energy and contain large resonance regions, making them computationally expensive to model with high fidelity. The multigroup method is a common approach used to model energy-dependent cross sections that splits the energy range into \( G \) finite regions, each with a representative cross section. The multigroup equations for \( G \) groups in 1D slab geometry in matrix form are\(^3\)

\[
\mathbf{\Sigma}(x) = \begin{pmatrix}
\Sigma_{1,1}(x) & 0 & \cdots & 0 \\
0 & \Sigma_{1,2}(x) & 0 & \cdots \\
\vdots & \ddots & \ddots & \vdots \\
0 & \cdots & 0 & \Sigma_{1,G}(x)
\end{pmatrix}, \quad (19)
\]

and

\[
\tilde{\psi} = (\psi_1, \psi_2, \ldots, \psi_G)^T, \quad \tilde{q} = (q_1, q_2, \ldots, q_G)^T, \quad (18)
\]

Fig. 2. 256 points generated in a unit square with pseudorandom points (top left), Sobol Sequence\(^{33}\) (top right), Halton Sequence\(^{34}\) (bottom left), and Golden Sequence\(^{32}\) (bottom right).
the experiments.

As a consequence of this energy discretization and the employed scattering-free particle tracing technique, each particle in the MC sweep can now represent all energy groups. Conversely, in analog MC, each simulated particle may represent only one energy group, and random samples are taken to determine up or down scattering after collision. In our hybrid iQMC method, the statistical weight of each particle is now a vector of weights, similar to Eq. (18):

$$\vec{w} = (w_1, w_2, \ldots, w_G)^T.$$  \hspace{1cm} (21)

Therefore, we only need to multiply this vector by the scattering cross section, Eq. (20), to determine the scattering distribution.

### III. IMPLEMENTATION DETAILS

The algorithm was written in Julia, a scientific computing language that combines the compiler capabilities of C++ and the syntax of Matlab and Python. The code and primary documentation are available here: https://github.com/spasmann/iQMC.jl (Ref. 36). The Krylov linear solvers come from the Julia package https://github.com/ctkelley/SIAMFANLEquations.jl (Ref. 37). The documentation for these codes is in the https://github.com/ctkelley/NotebookSIAMFANLJulia notebooks and the book that accompanies the package.

The results in Sec. IV were generated using the Sobol Sequence as the LDS in QMC Sweep. The Sobol Sequence generates nets with $2^n$ points and loses some of its balance properties if generated with a sample size that is not a power of 2 (Ref. 40). Consequently, the number of particles $N$ is varied by powers of 2 in all experiments. A brief convergence comparison among the Sobol, Halton, and Golden Sequences can be seen in problem 2 in Sec. IV.B, Fig. 9. Finally, for an equivalent comparison to MC, the LDS was replaced with a fixed-seed pseudorandom number generator. By fixed seed, we refer to a calculation where the random number seed is reset at the beginning of each iteration; this assures that the stochasticity of the MC algorithm is not an impediment to convergence. An outline of the QMC Sweep algorithm is described in Algorithm 1.

**Algorithm 1 QMC Sweep (\(\phi_{in}\))**

1: Initialize LDS
2: for \(i\) in \(N\) do
3: Assign position and angle \((x_i, \mu_i)\) based on the LDS
4: Initialize weight \(w_j = (\Sigma \phi_{in} + q)N_i V/N\)
5: for \(j\) in \(N_i\) do
6: Move particle across Zone \(j\)
7: Tally\((x, \mu, w)\) [Eq (13)]
8: Update particle weight [Eq. (12)]
9: end for
10: end for
11: Return: \(\phi_{out}\)

As previously mentioned in Sec. II, the described iQMC algorithm does not require the explicit formation of matrix \(A\) for the linear solver. Instead, we compute the matrix vector product \(A\phi\), as described in Algorithm 2, from which the Krylov Solvers can iterate.

**Algorithm 2 Matrix Vector Product (\(\phi_{in}\))**

1: \(b = \text{QMC Sweep}(\vec{0})\)
2: \(mxv = \text{QMC Sweep}(\phi_{in})\)
3: \(axv = \phi_{in} - mxv - b\)
4: Return: \(axv\)

To evaluate the effect of varying the number of spatial cells \(N_s\) within a QMC simulation, a postprocess spatial averaging technique was developed. Given a reference solution for the scalar flux with \(N_{sRef}\) spatial cells, experiments were run for problems 1 and 2 in Secs. IVA and IV.B, respectively, with \(N_s = (N_{sRef})^{2^n}\). The resulting vectors can be averaged \([\log(N_s/N_{sRef})]/\log(2)\] times to reduce all vectors to the length of the reference solution as seen in Algorithm 3.
To simulate an infinite medium, we placed an isotropic boundary source on each slab edge, where the source strength was held at the expected analytic solution. Figure 3 shows the center of each energy group for the total cross section against the analytic solution for scalar flux from Eq. (22) divided by the energy bin width.

From the convergence of relative residuals in Fig. 4, it is observed that the Krylov methods require far fewer transport sweeps to achieve the same levels of convergence as the SI regardless of the number of groups. Figure 5 plots the residual,

\[ R = \frac{||\phi_{\text{Sol}} - \phi_{\text{QMC}}||_\infty}{\phi_{\text{Sol}}} \]  

against the number of particle histories \( N \) for a given number of spatial cells \( N_r \) along with the theoretical convergence goal of \( O(N^{-1}) \) for QMC and \( O(N^{-1/2}) \) for MC.

Simulations were run with 80, 160, and 320 spatial cells, and afterward, results were run through the spatially averaged scalar flux postprocessing technique from Algorithm 3. This allows for comparison of all results to a solution \( \phi_{\text{Sol}} \) with \( N_r = 80 \). Because the solution is spatially constant per energy group, the results converge at the approximate rate of \( O(N^{-1}) \) for QMC and \( O(N^{-1/2}) \) for MC, regardless of the number of spatial cells (Fig. 5).

**IV.B. Problem 2: Reed’s Multimedia Problem**

The second problem, known as Reed’s Problem, is a monoenergetic multimedia problem in slab geometry.\(^{41}\) The problem features five unique media that are reflected across the problem for a total of nine regions; see Fig. 6. To ensure that each spatial cell contained only one medium, Reed’s Problem was run so that \( N_r \) was evenly divisible by 16, the range of the problem.

Reed’s Problem was benchmarked using results from an \( N = 10^{10} \) analog MC simulation from CEMeNT’s MCDC (Ref. 24). Additionally, in analyzing the relative error, it was observed that the solution to the problem approaches zero in multiple locations, and this was drastically increasing the relative error as reported in the previous problem. Instead, for Reed’s Problem we report the \( L_\infty \) norm of the error as seen in Eq. (24):
Fig. 4. Multigroup relative residuals defined as $||\Phi_n - \Phi_{n-1}||$ for (a) 12-group, (b) 70-group, and (c) 618-group problems with $N = 2048$.

Fig. 5. Relative error from the 12-group QMC and MC scalar flux results compared to analytic solution for varying number of particles $N$ and spatial cells $N_x$. The QMC results achieve the expected $O(N^{-1})$ convergence while the MC results converge at the standard $O(N^{-1/2})$. 
the convergence and QMC aged number 1 number outperform (\[\].

Problem 2048 Fig. \(s = 1\) beyond Sec. IV. The error of SCIENCE the number is reduced, the number of MC iterations, however, is nearly the same as the MC results because they did not reach the spatial error limit for \(N_x = 80\), near \(10^{-2}\).

Finally, Fig. 9 shows the results from a simulation with \(N_x = 80\) using the Sobol, Halton, and Golden Sequences and a pseudorandom number generator (MC). The MC results perform as expected, and the three LDSs perform rather similarly. The Golden Sequence achieves a lower error for the first few particle counts, but the Sobol Sequence results plateau at a lower error and ultimately achieve the greatest accuracy.

IV.C. Problem 3: Isotropic Boundary Source

The third and final computational experiment solves the monoenergetic problem from Garcia and Siewert,\(^{25}\) outlined in Table 1. Here, the scattering cross section is spatially dependent, defined by \(\Sigma_s = e^{-s/\bar{\Sigma}}\), and we considered two cases: \(s = 1\) and \(s = \infty\). Note that \(s = \infty\) is equivalent to a constant scattering cross section and therefore is the more difficult of the two scenarios as it involves more scattering and therefore more iterations for the scattering source to converge.

First, we solve the QMC linear problem with \(N = 2048\) particles and \(N_x = 100\) spatial cells. Similar to problems 1 and 2 in Secs. IV.A and IV.B, Fig. 10 shows that for an exponentially decaying scattering cross section (\(s = 1\)), the Krylov iterations take fewer than a third of the number of transport sweeps than that of SI for a relative residual of \(10^{-9}\). Figure 11 shows that for the constant scattering cross section, \(s = \infty\), the Krylov iterations took less than 25 iterations to reach a relative error of \(10^{-6}\) while SI required nearly 200 iterations.
IV.C.1. Validation and Calibration Study

We conclude this problem with a validation study given the results from Ref. 25 that are angular flux exit distributions accurate to six significant figures; see Fig. 12. We duplicated the results by obtaining the cell-average scalar flux from the QMC simulation, for $N = 2048$ and $N_x = 100$, and then used the scalar

$$\|\phi - \phi_0\|_\infty$$

of the absolute error of QMC scalar flux results compared to MCDC for varying number of particles $N$ and spatial cells $N_x$. The QMC results converge at $O(N^{-1})$ until limited by the spatial error. Increasing $N_x$ lowers the spatial error limit.

### Table I

Parameters for Fixed Boundary Source, Slab Geometry, and Simulation from Garcia and Siewert$^{25}$

| Parameter | Value |
|-----------|-------|
| $\Sigma_t$ | 1     |
| $\Sigma_s(x)$ | $e^{-x/s}$ |
| $r$ | 5     |
| $\psi_l(\mu)$ | 1     |
| $\psi_r(\mu)$ | 0     |
| $N_x$ | 50    |
| $q(x)$ | 0     |

Fig. 10. Scalar flux relative residuals for $s = 1$ given parameters from Table I and $N = 2048$ and $N_x = 100$. 

Fig. 9. Comparison of the Sobol, Halton, and Golden Sequences along with results from a pseudorandom number generator for $N_x = 80$. The Golden Sequence achieves the best accuracy for low particle histories but is eventually outperformed by the Sobol Sequence.

Fig. 8. $L_\infty$ of the absolute error of QMC scalar flux results compared to MCDC for varying number of particles $N$ and spatial cells $N_x$. The QMC results converge at $O(N^{-1})$ until limited by the spatial error. Increasing $N_x$ lowers the spatial error limit.
flux as the input for a single $S_N$ transport sweep (with scattering treated as an internal source term) to recover the exit distributions. We report the corresponding results from Ref. 25 in Tables II and III. As is clear from Table II, the exit distributions can vary by five orders of magnitude. The results from QMC agree with the benchmarks to roughly two significant figures.

In Tables IV and V, we look at the relative errors $R$, Eqs. (25), (26), and (27), in the QMC exit distributions as compared to a highly accurate $S_N$ result:

$$ R = \max(R^0, R^r), \quad (25) $$

where

$$ R^0 = \max_{\mu} \left| \frac{\psi^{SN}(0, -\mu) - \psi^{OMC}(0, -\mu)}{\psi^{SN}(0, -\mu)} \right| $$

and

$$ R^r = \max_{\mu} \left| \frac{\psi^{SN}(\tau, \mu) - \psi^{OMC}(\tau, \mu)}{\psi^{SN}(\tau, \mu)} \right|. \quad (27) $$

We compensate for the widely varying scales by tabulating, for each value of $N$ and $N_x$. Finally, similar to the previous two problems, we plot the residual $R$ for

Fig. 11. Scalar flux relative residuals for $s = \infty$ given parameters from Table I and $N = 2048$ and $N_x = 100$.

Fig. 12. Angular flux exit distributions provided by Garcia and Siewert. Recreated using scalar flux data from QMC and subsequent angular flux exit distributions from an $S_N$ approximation.
### TABLE II
Angular Flux Exit Distributions from Garcia and Siewert and the $S_N$ QMC Sweep for $s = 1^*$

| $\mu$ | Garcia and Siewert | QMC |
|-------|---------------------|-----|
|       | $\psi(0, -\mu)$    | $\psi(\tau, \mu)$ | $\psi(0, -\mu)$ | $\psi(\tau, \mu)$ |
| 0.05  | 5.8966e-01         | 6.0748e-06       | 6.0703e-01      | 5.9190e-06       |
| 0.10  | 5.3112e-01         | 6.9251e-06       | 5.4746e-01      | 6.7407e-06       |
| 0.20  | 4.4328e-01         | 9.6423e-06       | 4.5706e-01      | 9.3545e-06       |
| 0.30  | 3.8030e-01         | 1.6233e-05       | 3.9222e-01      | 1.5610e-05       |
| 0.40  | 3.3296e-01         | 4.3858e-05       | 3.4348e-01      | 4.1372e-05       |
| 0.50  | 2.9609e-01         | 1.6937e-04       | 3.0551e-01      | 1.5862e-04       |
| 0.60  | 2.6656e-01         | 5.7346e-04       | 2.7509e-01      | 5.3951e-04       |
| 0.70  | 2.4239e-01         | 1.5128e-03       | 2.5019e-01      | 1.4325e-03       |
| 0.80  | 2.2235e-01         | 3.2436e-03       | 2.2942e-01      | 3.0897e-03       |
| 0.90  | 2.0517e-01         | 5.9603e-03       | 2.1183e-01      | 5.7055e-03       |
| 1.00  | 1.9054e-01         | 9.7712e-03       | 1.9675e-01      | 9.3919e-03       |

*With $N = 2048$ and $N_c = 100$.

### TABLE III
Angular Flux Exit Distributions from Garcia and Siewert and the $S_N$ QMC Sweep for $s = \infty^*$

| $\mu$ | Garcia and Siewert | QMC |
|-------|---------------------|-----|
|       | $\psi(0, -\mu)$    | $\psi(\tau, \mu)$ | $\psi(0, -\mu)$ | $\psi(\tau, \mu)$ |
| 0.05  | 8.9779e-01         | 1.0220e-01       | 9.0605e-01      | 1.0368e-01       |
| 0.10  | 8.8783e-01         | 1.1216e-01       | 8.9584e-01      | 1.1369e-01       |
| 0.20  | 8.6958e-01         | 1.3041e-01       | 8.7648e-01      | 1.3190e-01       |
| 0.30  | 8.5229e-01         | 1.4770e-01       | 8.5893e-01      | 1.4924e-01       |
| 0.40  | 8.3550e-01         | 1.6449e-01       | 8.4219e-01      | 1.6612e-01       |
| 0.50  | 8.1899e-01         | 1.8100e-01       | 8.2587e-01      | 1.8273e-01       |
| 0.60  | 8.0267e-01         | 1.9732e-01       | 8.0978e-01      | 1.9915e-01       |
| 0.70  | 7.8649e-01         | 2.1350e-01       | 7.9383e-01      | 2.1542e-01       |
| 0.80  | 7.7042e-01         | 2.2957e-01       | 7.7799e-01      | 2.3158e-01       |
| 0.90  | 7.5449e-01         | 2.4550e-01       | 7.6226e-01      | 2.4754e-01       |
| 1.00  | 7.3872e-01         | 2.6127e-01       | 7.4667e-01      | 2.6336e-01       |

*With $N = 2048$ and $N_c = 100$.

### TABLE IV
Exit Distribution Errors, $R$: $s = 1.0$, for Varying the Number of Spatial Cells, $N_c$, and Particles per Transport Sweep, $N$

| $N_c$ | $N$ | 1024 | 2048 | 4096 | 8192 | 16 384 |
|------|-----|------|------|------|------|--------|
| 50   | 1.3697e-01 | 1.3426e-01 | 1.3512e-01 | 1.3532e-01 | 1.3524e-01 |
| 100  | 6.0963e-02 | 6.3576e-02 | 6.4619e-02 | 6.4889e-02 | 6.4853e-02 |
| 200  | 3.7722e-02 | 3.1249e-02 | 3.1200e-02 | 3.1733e-02 | 3.1671e-02 |
| 400  | 1.7131e-02 | 1.5261e-02 | 1.9622e-02 | 7.5686e-03 | 7.1669e-03 |
| 800  | 9.5855e-03 | 1.0178e-02 | 1.9304e-02 | 7.5686e-03 | 7.1669e-03 |
| 1600 | 7.1871e-03 | 1.2087e-02 | 2.1951e-02 | 3.6351e-03 | 3.8520e-03 |
| 3200 | 5.1113e-03 | 1.2892e-02 | 2.1984e-02 | 2.3673e-03 | 1.8255e-03 |
varying $N$ and $N_x$ in Fig. 13. However, unlike the previous two problems, the scalar flux averaging algorithm was not applied. In the QMC case of $s = 1.0$, we notice that if the number of spatial cells is increased with the number of particles, the $O(N^{-1})$ convergence is achieved. For $s = \infty$, the QMC results converge irrespective of the number of spatial cells.

**Table V**

| $N_x$ | $N$  | 1024     | 2048     | 4096     | 8192     | 16384    |
|-------|------|----------|----------|----------|----------|----------|
| 50    | 2.83725e-02 | 1.22374e-02 | 1.19906e-02 | 1.15398e-02 | 1.15951e-02 |
| 100   | 2.41784e-02 | 1.53219e-02 | 6.81242e-03 | 5.67372e-03 | 5.90660e-03 |
| 200   | 1.95960e-02 | 1.32236e-02 | 6.73505e-03 | 2.37596e-03 | 2.91740e-03 |
| 400   | 1.86114e-02 | 1.37280e-02 | 1.04038e-02 | 1.07665e-03 | 1.63724e-03 |
| 800   | 3.02170e-02 | 1.15453e-03 | 1.21401e-02 | 1.37999e-03 | 1.13099e-03 |
| 1600  | 2.26681e-02 | 3.93529e-02 | 1.78938e-02 | 1.71729e-03 | 1.17343e-03 |
| 3200  | 3.30886e-02 | 5.40682e-02 | 2.52993e-02 | 1.48919e-03 | 1.51562e-03 |

Fig. 13. Relative error of fixed-seed QMC and MC results for $s = 1$ and $s = \infty$ compared to $S_n$ solution for varying number of particles $N$ and spatial cells $N_x$. Increasing the spatial cells and particle count simultaneously in QMC simulations achieves $O(N^{-1})$ convergence.
V. CONCLUSION

We have described the general-purpose iQMC method for solving the NTE. The use of iterative solvers and a continuous weight absorption technique provides a well-suited application for QMC that provides an enhanced convergence rate of $O(N^{-1})$ compared to the $O(N^{1/2})$ of standard MC simulation. Additionally, the use of advanced iterative solvers like the Krylov methods GMRES and BiCGSTAB provides greatly increased convergence of residuals. The benefits of this algorithm were observed on all three 1D test problems where the hybrid method provided both more accurate and efficient solutions. Future work will look to see if these benefits are maintained on more difficult and complex problems including criticality eigenvalue, time-dependent, 2D, and three-dimensional problems. The massive parallelism inherent in MC combined with iQMC's particle tracing and vectorized multigroup methods suggests that it would benefit greatly from parallel implementation on advanced architectures and GPUs.

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