Center for Exascale Monte Carlo Neutron Transport

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Sam Pasmann: iQMC: The iterative Quasi-Monte Carlo Method for Neutron Transport

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Abstract

Iterative Quasi-Monte Carlo (iQMC) is a new method for computational neutron transport. iQMC replaces standard quadrature techniques used in deterministic linear solvers with Quasi-Monte Carlo simulation for more accurate and efficient solutions to the neutron transport equation. Quasi-Monte Carlo (QMC) is the use of low-discrepancy sequences to sample the phase space in place of pseudo-random number generators. 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 neutron transport equation (NTE) can be modeled as a pure-absorption problem. This removes the need to explicitly model particle scattering/fission processes and reduces the MC simulation to a 'ray tracing' process. The ray trace transport sweep provides an application well-suited for QMC and for computation on GPUs.

In addition to standard linear solvers like the source iteration, iQMC takes advantage of Krylov solvers like GMRES which require far fewer transport sweeps for convergence. To date, iQMC has been implemented in the Monte-Carlo Dynamic Code (MC/DC) and has achieved a $O(1/N)$ convergence rate on several 1D, 2D, and 3D multigroup problems.

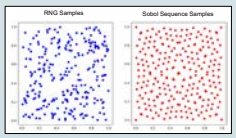
Introduction

High fidelity simulation of a nuclear reactor core, particularly in complex transient scenarios, is a central goal in computational nuclear engineering. This goal has remained largely out-of-reach due to the immense computational cost associated with these simulations given current hardware and algorithmic limitations. However, with the continuous deployment of faster and more powerful computers, like Lawrence Livermore National Laboratories' *El Capitan*, the era of exascale computing (defined as 10^{18} floating point operations per second) has arrived [1]. The increase in computational power and a shifting landscape from computing primarily on CPUs to GPUs provides motivation to develop new computational methods that can better leverage available resources.

The Center for Exascale Monte Carlo for Neutron Transport (CEMeNT) [2] is a collaborative effort between Oregon State University, North Carolina State University, and the University of Notre Dame. The goal of the center is to advance Monte Carlo neutron transport capabilities on problems relevant to the National Nuclear Security Administration's (NNSA) mission via three main thrusts:

- Computational physics and simulation of time-dependent neutron transport phenomena
- Exascale software engineering
- Predictive science

To help accomplish this goal, we have designed a hybrid deterministic-Monte Carlo algorithm. This algorithm uses deterministic iterative methods and Quasi-Monte Carlo simulation to increase the convergence rate regularly associated with Monte Carlo simulation and provide an algorithm better tailored for computation on GPUs.



256 points plotted in a unit-square from a typical pseudo-random number generator and the Sobol Sequence (a popular low-discrepancy sequence). The Sobol sequence samples the phase space in a more uniform manner leading to a better approximation with fewer samples.

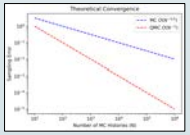
Methodology

The core ideas behind the iterative Quasi-Monte Carlo Method:

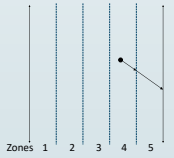
Deterministic Iterative Methods	• We use deterministic linear iterative methods to iterate on the scattering and fission terms • In addition to standard iterative solvers like the source iteration we can also utilize Krylov solvers like GMRES
+	
Monte Carlo for Neutron Transport	• Typical quadrature techniques are replaced with Monte Carlo simulation • We no longer explicitly model particle scattering/fission • The MC simulation essentially becomes a 'ray trace'
+	
Quasi-Monte Carlo	• The ray tracing process provides a well-suited application of QMC • The low-discrepancy nature of QMC allows the use of a fixed-seed iterative process • QMC provides enhanced convergence rate

The QMC Sweep

Quasi-Monte Carlo simulation forms the basis linear solvers. By removing the need to explicitly model the scattering and fission processes, the system can be treated as a pure-absorber where each particle is given an angle, position, and statistical weight. The initial position and angle are generated from the LDS, while the initial weight is calculated via the RHS of the NTE. After a particle is born, it is traced or *swept* out of the volume. The sweep is greatly enhanced with the use of a continuous weight reduction technique which, reduces the statistical weight of the particle per path length traveled. Then a path-length tally estimator is used to compute the spatially-averaged scalar flux in each zone of the defined mesh. iQMC utilizes a multigroup energy discretization, consequently each simulated particle can now represent all energy groups. As the particle is traced out of the volume, each energy group can be attenuated in parallel [3].



Theoretical convergence of Monte Carlo and Quasi-Monte Carlo sampling on a log-log scale. Note, when $N = 10^6$ QMC is more than three orders of magnitude more accurate than MC.



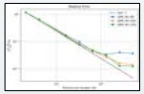
A simplified diagram of a Monte Carlo sweep in an infinite slab. For each MC sweep the particles are emitted with initial position and angle and are swept out of the volume, tallying the scalar flux according to a path length tally estimator.

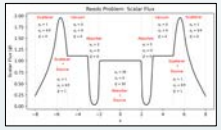
Results

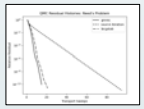
Implementation

iQMC was implemented and verified in the Monte Carlo Dynamic Code (MC/DC) a performant, scalable, and machine-portable Python-based Monte Carlo neutron transport software currently in development in CEMeNT [4]. MC/DC takes advantage of *Numba* [5], a just-in-time compiler for scientific computing in Python which has been shown to provide 56-212x speedups over pure Python on various reactor problems.

Fixed Source Problems



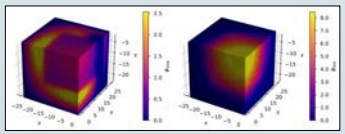




Reed's problem is a 1D multi-region slab geometry [6]. The Krylov solvers far outperform Source Iteration, requiring no less than one-quarter the number of iterations to converge. The effects of increasing the number of spatial cells (N_c) are clearly seen as the relative error plateaus. Our QMC sweep currently utilizes a flat source for each cell, and beyond a certain number of particle histories N, the convergence is limited by spatial error determined by N_c. As the number of spatial cells is increased, the spatial error is reduced and the QMC can continue to converge at the $O(N^{-1})$ rate.

k-Eigenvalue Problems

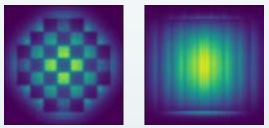
iQMC has also been demonstrated [7] to solve k-eigenvalue problems MC/DC. Scalar flux results are shown from the 3-D, 2-group, Takeda-1 Benchmark problem [8]. iQMC achieved the expected $O(N^{-1})$ convergence rate of the scalar flux with both the power iteration and Davidson method (a Krylov solver). The Davidson method was shown to be a valuable tool for solving for the dominant eigenvalue, requiring as few as 1/2 the number of transport sweeps for convergence of the eigenvalue than the power iteration.



Conclusions and Ongoing Work

iQMC is an iterative Quasi Monte Carlo method for neutron transport. Computational experiments have shown iQMC to achieve an approximate convergence rate of $O(N^{-1})$ compared to the typical $O(N^{-1/2})$ of typical Monte Carlo simulation. To fully assess iQMC as a next-generation neutron transport solver, the method will need to be developed to encompass time-dependent calculations, at-scale on modern CPU and GPU hardware, on a difficult full-scale transient reactor problem. To accomplish this, the following work remains:

- Reducing the spatial discretization error i.e. "teleportation error" (in progress)
- Development of a time-dependent algorithm
- Development of MC/DC for GPU computation



Scalar flux results from an analog MC simulation of a time-dependent SMR challenge problem designed by CEMeNT. This problem will be iQMC's final test, which we can then compare performance between analog MC and other variance reduction techniques.

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Acknowledgements

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