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A Comparison of Monte Carlo Particle Transport Algorithms for an Interior Source Binary Stochastic Medium Benchmark Suite

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INTRODUCTION

Particle transport through binary stochastic mixtures has received considerable research attention in the last two decades [1]. Zimmerman and Adams [2] proposed a Monte Carlo algorithm (Algorithm A) that solves the Levermore-Pomraning equations [1] and another Monte Carlo algorithm (Algorithm B) that should be more accurate as a result of improved local material realization modeling. Zimmerman and Adams [2] numerically confirmed these aspects of the Monte Carlo algorithms by comparing the reflection and transmission values computed using these algorithms to a standard suite of planar geometry binary stochastic mixture benchmark transport solutions [3]. The benchmark transport problems are driven by an isotropic angular flux incident on one boundary of a binary Markovian statistical planar geometry medium.

In a recent paper [4], we extended the benchmark comparisons of these Monte Carlo algorithms to include the scalar flux distributions produced. This comparison is important, because as demonstrated in Ref. [5], an approximate model that gives accurate reflection and transmission probabilities can produce unphysical scalar flux distributions. Brantley and Palmer [6] recently investigated the accuracy of the Levermore-Pomraning model using a new interior source binary stochastic medium benchmark problem suite. In this paper, we further investigate the accuracy of the Monte Carlo algorithms proposed by Zimmerman and Adams by comparing to the benchmark results from the interior source binary stochastic medium benchmark suite [6], including scalar flux distributions. Because the interior source scalar flux distributions are of an inherently different character than the distributions obtained for the incident angular flux benchmark problems, the present benchmark comparison extends the domain of problems for which the accuracy of these Monte Carlo algorithms has been investigated.

BENCHMARK TRANSPORT PROBLEMS

We consider the following time-independent monoenergetic neutron transport problem with isotropic scattering in a one-dimensional planar geometry spatial domain defined on $0 \leq x \leq L$:

$$\mu \frac{\partial}{\partial x} \psi(x,\mu) + \sigma_t(x)\,\psi(x,\mu) = \frac{1}{2}\sigma_s(x) \int_{-1}^{1} \psi(x,\mu')\,d\mu' + \frac{1}{2} q(x) \quad ,$$

$$0 \leq x \leq L \ , \ -1 \leq \mu \leq 1 \ , \tag{1a}$$

$$q(x) = \frac{1}{L} \ , \ 0 \leq x \leq L \ , \tag{1b}$$

$$\psi(0,\mu) = 0 \ , \ \mu > 0 \ , \tag{1c}$$

$$\psi(L,\mu) = 0 \ , \ \mu < 0 \ . \tag{1d}$$

Eqs. (1) are written in standard neutronics notation [7]. The interior source defined by Eq. (1b) is non-stochastic, spatially uniform, and results in one neutron sourced into the medium per unit time. The vacuum boundary conditions given by Eqs. (1c) and (1d) are non-stochastic. The stochastic spatial medium is assumed to be composed of alternating slabs of two materials, labeled with the indices 0 and 1, with the mean material slab width for material i denoted as Λ_i. The total and scattering cross sections for each material are uniform and are denoted as σ_t^i and σ_s^i, i = 0, 1, respectively. The distribution of material slab widths in the planar medium is assumed to be described by spatially homogeneous Markovian statistics [1].

The material parameters for the benchmark transport problems are given in Table I using the notation of Ref. [5]. The scattering ratio for material i is defined as $c_i = \sigma_s^i/\sigma_t^i$. For each set of material parameters (cases 1, 2, and 3), three sets of scattering ratio combinations (cases a, b, and c) and three slab widths (L = 0.1, 1.0, and 10.0) are considered. The ensemble-averaged total cross section is unity for all cases. The different case numbers (i.e. 1, 2, and 3) represent permutations of materials with mean material slab widths of optical depth 0.1, 1.0, and 10.0. The different case letters (i.e. a, b, and c) represent varying amounts of scattering for each material.

One fiducial comparison quantity is the ensemble-averaged leakage from the slab at x = 0, $\langle J_0 \rangle$, defined as

$$\langle J_0 \rangle = \int_{-1}^{0} |\mu| \langle \psi(0,\mu) \rangle \, d\mu \ . \tag{2}$$

(In the limit of an infinite number of realizations, the leakage at the left and right boundaries of the slab should be identical. Given the finite number of realizations used in the generation of our benchmark results, we choose to simply compare the leakage from the slab at x = 0, $\langle J_0 \rangle$.) In addition, we compare the ensemble-averaged material scalar flux distributions, $\langle \phi_i(x) \rangle$, i = 0, 1, as these distributions determine reaction rates in the system.

Table I. Material Parameters for Benchmark Transport Problems

Case	σ_t^0	Λ_0	σ_t^1	Λ_1	Case	c_0	c_1	L
1	10/99	99/100	100/11	11/100	a	0.0	1.0	0.1
2	10/99	99/10	100/11	11/10	b	1.0	0.0	1.0
3	2/101	101/20	200/101	101/20	c	0.9	0.9	10.0

MONTE CARLO ALGORITHMS

For both Algorithms A and B, a particle history begins with sampling the source particle characteristics including a material identifier for the particle. Distances to the required events are then either sampled or computed. The distance to collision, d_c, is sampled using the macroscopic total cross section corresponding to the material in which the particle exists. Because we are interested in comparing the material scalar flux distributions, we impose a uniform spatial mesh on the spatial domain in which to tally this information using a track length estimator [7]. As a result, we introduce a new distance calculation, the distance to zone boundary, d_b, computed using the current position and direction of flight of the particle and the boundaries of the spatial zone in which the particle exists. For both Monte Carlo algorithms, the distance the particle travels in the zone is tallied whenever the particle is moved. In the next sections, we describe in more detail the particle history flow for Algorithms A and B.

Algorithm A: The Levermore-Pomraning Solution

For each particle history:

1. Compute d_b and sample d_c as described above.
2. Sample the distance to material interface, d_i, by sampling a material slab width from Markovian statistics and dividing by the particle direction cosine to account for the direction of particle motion.
3. Compute the minimum of d_b, d_c, and d_i to determine the sampled event.
4. If d_b is the minimum distance, move the particle to the zone boundary. If the particle is escaping the spatial domain, update the appropriate leakage tally, terminate the history, and track the next particle. Otherwise, return to step 1.
5. If d_c is the minimum distance, move the particle the appropriate distance, and sample the collision type using the macroscopic total and scattering cross sections for the material in which the particle exists. If the sampled collision is absorption, terminate the history and track the next particle. If the sampled collision is scattering, perform the scattering collision by sampling the outgoing characteristics of the scattered particle; the particle maintains its current material identifier. Return to step 1.
6. If d_i is the minimum distance, move the particle the appropriate distance and switch the material identifier. Return to step 1.

Note that following a collision, a new distance to material interface is sampled. As a result, the particle encounters a different material realization following a collision, which is unphysical. As noted by Zimmerman and Adams [2], this algorithm is exact in a purely absorbing medium. We expect Algorithm A to be less accurate in highly scattering materials with optically thick mean material slab widths. Because we have imposed a spatial mesh on the problem, a new distance to material interface is also sampled following a zone boundary crossing. Since Algorithm A models a Markovian (i.e. a no-memory) transport process involving uncorrelated particle flights, sampling a new distance to material interface following a zone boundary crossing does not introduce additional error into the algorithm.

Algorithm B: A More Accurate Solution

For each particle history:

1. Sample the distance to material interface values in the forward and backward directions of particle motion, d_i^+ and d_i^-, respectively, as described in Algorithm A.
2. Compute d_b and sample d_c as described above.
3. Compute the minimum of d_b, d_c, and d_i^+ to determine the sampled event.
4. If d_b is the minimum distance, initially treat as in Algorithm A. In addition, adjust the distance to material interface values in the forward and backward directions to account for the distance the particle was moved. Return to step 2.
5. If d_c is the minimum distance, initially treat as in Algorithm A. In addition, adjust the distance to material interface values in the forward and backward directions to account for the distance the particle was moved. If the sampled collision is scattering, also adjust the distance to material interface values in the forward and backward directions to account for the change in direction of flight of the particle after the scatter. Switch the forward and backward distance to material interface values if the particle is backscattered. Return to step 2.

6. If d_i^+ is the minimum distance, move the particle the appropriate distance, switch the material identifier, sample a new d_i^+, and set d_i^- to zero. Return to step 2.

In Algorithm B, a particle can move within one material and encounter the same realization, which is more physically realistic than Algorithm A. As a result, we expect Algorithm B to be more accurate than Algorithm A.

NUMERICAL RESULTS

We computed Monte Carlo solutions for the interior source benchmark problem suite using both Algorithms A and B. We tallied the Monte Carlo scalar flux distributions using 100 uniform spatial zones. Each Monte Carlo simulation was performed using 10^9 particle histories, resulting in pointwise relative standard deviations for the material scalar flux distributions of less than 0.1% in all cases. We focus here on the L = 10 slab width results, as the largest errors occur for this slab width.

Table II presents for each of the nine material/scattering ratio cases the relative error in the computed leakage and the root-mean-squared relative error in the computed ensemble-averaged scalar flux distributions compared to the benchmark results [6]. Overall, we find that Algorithm B generally produces significantly more accurate leakage values than Algorithm A and also significantly more accurate material scalar flux distributions. Both Monte Carlo transport algorithms robustly produce physically-realistic scalar flux distributions for the transport problems examined. These conclusions are generally consistent with results from the incident angular flux benchmark suite [2, 4].

The largest error in the scalar flux distributions occurs in case 2a. The material zero scalar flux computed by Algorithm A for this case is reasonably accurate (RMS relative error of 2.5%), while the material one scalar flux distribution exhibits large pointwise errors (RMS relative error of 61.9%). For this case, materials zero and one have mean material slab widths of one and ten, respectively. Material one is purely scattering and optically thick, conditions under which the Levermore-Pomraning model (Algorithm A) is known to be only approximate. Material zero is purely absorbing, and hence Algorithm A should be generally accurate in this material. Algorithm B produces significantly more accurate scalar flux distributions for this case.

Table II. Summary of Numerical Results for L = 10

			(RMS) Relative Error	
Case	Case	Quantity	Algorithm A	Algorithm B
1	a	$\langle J_0 \rangle$	0.085	0.054
		$\langle \phi_0 \rangle$	0.047	0.031
		$\langle \phi_1 \rangle$	0.108	0.082
	b	$\langle J_0 \rangle$	-0.052	-0.012
		$\langle \phi_0 \rangle$	0.064	0.009
		$\langle \phi_1 \rangle$	0.012	0.004
	c	$\langle J_0 \rangle$	-0.012	-0.004
		$\langle \phi_0 \rangle$	0.149	0.086
		$\langle \phi_1 \rangle$	0.043	0.040
2	a	$\langle J_0 \rangle$	0.024	0.015
		$\langle \phi_0 \rangle$	0.025	0.013
		$\langle \phi_1 \rangle$	0.619	0.073
	b	$\langle J_0 \rangle$	-0.085	-0.001
		$\langle \phi_0 \rangle$	0.082	0.002
		$\langle \phi_1 \rangle$	0.137	0.008
	c	$\langle J_0 \rangle$	-0.094	-0.004
		$\langle \phi_0 \rangle$	0.145	0.018
		$\langle \phi_1 \rangle$	0.314	0.039
3	a	$\langle J_0 \rangle$	-0.005	0.010
		$\langle \phi_0 \rangle$	0.101	0.078
		$\langle \phi_1 \rangle$	0.432	0.108
	b	$\langle J_0 \rangle$	-0.030	-0.002
		$\langle \phi_0 \rangle$	0.018	0.016
		$\langle \phi_1 \rangle$	0.012	0.004
	c	$\langle J_0 \rangle$	-0.062	0.000
		$\langle \phi_0 \rangle$	0.146	0.037
		$\langle \phi_1 \rangle$	0.063	0.023

CONCLUSIONS

We have numerically investigated the accuracy of two Monte Carlo algorithms originally proposed by Zimmerman and Adams [2] for particle transport through a binary stochastic mixture using an interior source planar geometry benchmark suite [6]. Both Algorithms A and B produce qualitatively and semi-quantitatively correct results for the leakage values and the scalar flux distributions for this interior source benchmark suite. Overall, we find that Algorithm B is significantly more accurate than Algorithm A. These conclusions are consistent with the results of previous research [2, 4] investigating the accuracy of these Monte Carlo algorithms using an incident angular flux benchmark suite.

The material parameters used in the benchmark suite examined in this work are the same as used in previous incident angular flux benchmark suite investigations [2–5]. For some mean material slab width and total slab width values used in the benchmark suite, a small number of distinct material slabs are present in typical realizations (although some realizations have significantly larger numbers). Examining additional ranges of material parameters and larger slab widths may be beneficial in further assessing the relative accuracy of Algorithms A and B.

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