INTRODUCTION

The material properties at a given spatial location are known only statistically in a stochastic medium [1]. The most common approach to solving particle transport problems involving binary stochastic media is to use the atomic mix (AM) approximation [1] in which the transport problem is solved using ensemble-averaged (homogenized) material properties. A common deterministic model developed for solving particle transport problems in binary stochastic media is the Levermore-Pomraning (LP) model [1, 2]. Adams et al. [3] investigated the accuracy of the LP model in one-dimensional (1D) planar geometry by comparing LP solutions to benchmark solutions obtained by sampling large numbers of material realizations using Markovian statistics, solving a transport problem for each realization, and ensemble averaging the results. Zimmerman and Adams [4] proposed a Monte Carlo LP algorithm that produces the Levermore-Pomraning solution and another local realization preserving (LRP) algorithm that typically improves accuracy by locally preserving the material realization encountered by the Monte Carlo particle. These algorithms have been extensively studied using 1D planar geometry benchmark investigations [4, 5]. The Monte Carlo LP algorithm is generally more accurate than the AM approximation, and the LRP algorithm is generally more accurate than both the AM and LP approximations. The Monte Carlo LP and LRP algorithms have been extended for use in thermal photon implicit Monte Carlo (IMC) applications [6, 7]. Benchmark comparisons in 1D planar geometry demonstrate that the LRP algorithm is generally more accurate than the LP algorithm for these thermal photon transport problems.

A significant limitation of these previous benchmark comparisons is the restriction to 1D planar geometry. Brantley and Martos [8] generated three-dimensional (3D) binary stochastic medium benchmark results for a particle transport problem with varying spherical inclusion mean chord lengths and three different spherical radius distributions. That research was an initial effort toward generating 3D benchmark results relevant to particle transport through a stochastic medium composed of inclusions of varying size and shape such as may be encountered in a turbulent medium. An example material realization from that research is shown in Fig. 1(a). (The range of material properties considered in that work was smaller than in the 1D benchmark studies.) Brantley [9] subsequently investigated the accuracy of a 3D Monte Carlo LP algorithm for these 3D benchmark problems (for the exponential spherical radius distribution case) and found that the LP approximation is significantly more accurate than the AM approximation. In addition, the LP approximation qualitatively captures trends in the solution that are not captured by the AM approximation.

A limitation of these previous 3D benchmark comparisons is that the chord length distribution in the background material and spherical inclusions is not exponential as assumed by the Monte Carlo LP approximation. As a result, the conclusions from that work regarding the accuracy of the LP approximation include both the effect of approximately treating the stochastic medium as well as the effect of inconsistent statistical distributions assumed in the Monte Carlo transport algorithm compared to that used to generate the stochastic medium realizations. Larmier et al. [10] have recently produced benchmark transport results for general d-dimensional Markovian binary stochastic media in which the chord length distributions in the materials are truly exponential. They considered the same material properties as Adams et al. [3], Zimmerman and Adams [4], and Brantley [5]. An example 3D material realization (from Ref. [10]) is shown in Fig. 1(b).

In this work, we extend previous 1D planar geometry studies [4, 5] by investigating the accuracy of 3D Monte Carlo AM, LP, and LRP algorithms using the benchmark results of Larmier et al. [10]. A detailed comparison of the benchmark and LP results has recently been performed [11]. Here we focus on the question of whether the LRP algorithm produces improved accuracy over the LP algorithm in 3D geometry as previously observed in 1D geometry.

### BINARY STOCHASTIC MEDIUM BENCHMARK PROBLEM SUITE

Larmier et al. [10] considered the following time-independent monoenergetic particle transport problem with isotropic scattering in a three-dimensional cubic spatial domain $D$ defined by $0 \leq x, y, z \leq L$ with outer boundary $\partial D$:

$$
\Omega \cdot \nabla \psi (x, \Omega) + \sigma_t(x) \psi (x, \Omega) = \frac{\sigma_s(x)}{4\pi} \int_{4\pi} \psi (x, \Omega') d\Omega', \quad (1a)
$$

$$
\psi (x, y, z = 0, \Omega) = \frac{1}{2\pi}, \quad 0 \leq x, y \leq L, \quad \Omega \cdot n < 0, \quad (1b)
$$
\[ \psi(x, y, z = L, \Omega) = 0, \quad 0 \leq x, y \leq L, \quad \nabla \cdot \mathbf{n} < 0. \quad (1c) \]

Here we have used standard particle transport notation [12]: \( \psi \) is the angular flux of particles [#/cm²-s-steradian] at a position \( x = (x, y, z) \) traveling in direction \( \Omega \); \( \sigma_t(x) \) is the macroscopic total cross section [cm⁻¹] at position \( x \); and \( \sigma_s(x) \) is the macroscopic scattering cross section [cm⁻¹] at position \( x \). Because the cross sections are random variables, the angular flux is also a random variable. An isotropic angular flux with unity incoming current is incident on the left edge of the domain at \( z = 0 \), where \( \mathbf{n} \) is the unit outer normal to \( \partial D \) at a position \( x \) on the boundary. A vacuum boundary condition is imposed on the right edge of the domain at \( z = L \). The boundaries on all other transverse edges of the cubic domain are reflecting. The benchmark ensemble-averaged fiducial quantities of interest are the reflection and transmission, given by

\[ R = \int_0^L \int_0^L \int_{\Omega > 0} \frac{\Omega \cdot \mathbf{n}}{\Omega \cdot \mathbf{n}} \psi(x, y, z = 0, \Omega) d\Omega dx dy, \quad (2) \]

and

\[ T = \int_0^L \int_0^L \int_{\Omega > 0} \frac{\Omega \cdot \mathbf{n}}{\Omega \cdot \mathbf{n}} \psi(x, y, z = L, \Omega) d\Omega dx dy, \quad (3) \]

respectively, where \( \mathbf{n} \) is the unit outer normal to \( \partial D \) at a position \( x \) on the boundary.

The suite of binary stochastic medium transport problems is characterized by the material properties given in Table 1 [3, 4, 5, 10]. All problems in the suite assume a spatial extent of \( L = 10 \). Material zero is an optically thin background matrix material, material one is an optically thick inclusion material, and \( \Lambda_i \) is the mean chord length for material \( i \). The scattering ratio of each material is given by \( c_i = \sigma'_s / \sigma_t \). The different case numbers (i.e., 1, 2, and 3) represent permutations of materials with mean chord lengths of optical depth (\( \sigma'_t \Lambda_i \)) 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. The probability of material \( i \) being present at a point in space, \( p_i \), is given by \( p_i = \Lambda_i / (\Lambda_0 + \Lambda_1) \).

**MONTE CARLO ALGORITHMS**

A detailed description of the Monte Carlo LP and LRP algorithms for 1D planar geometries is given in Ref. [5]. The extension to 3D geometries is relatively straightforward and has previously been described for the LP case [9]. Much of the standard Monte Carlo particle transport algorithm using the atom mix approximation is unaltered by the introduction of algorithms to model transport through a stochastic medium. A Monte Carlo particle must maintain an additional identifier describing the material in which the particle is currently located. This material identifier must be appropriately sampled (in proportion to the material volume fraction) when a particle is created from an external source or enters the problem from an external boundary. A particle history begins with sampling the source particle characteristics appropriately, including sampling the material identifier for the particle. In addition to standard events sampled during the Monte Carlo transport algorithm, a new event, the distance to material interface, \( d_i \), is introduced for Monte Carlo transport algorithms in stochastic media. We assume that the material chord lengths are distributed according to spatially homogeneous Markovian statistics [1], in which case the chord length values for material \( i \), \( \lambda_i \), follow an exponential distribution given by

\[ f_i(\lambda) = \frac{1}{\lambda_i} \exp \left( -\frac{\lambda}{\lambda_i} \right), \quad (4) \]

where \( \lambda_i \) is the mean chord length for material \( i \). A distance to material interface is sampled by sampling a material chord length from the exponential distribution given by Eq. (4), i.e., \( d_i = -\Lambda_i \ln(\xi) \), where \( \xi \) is a random number. This sampling of a distance to material interface models the material coupling term in the LP model. Next, distances to the other required standard Monte Carlo events are either sampled or computed. The distance to collision, \( d_c \), must be sampled using the macroscopic total cross section corresponding to the material in which the particle is located, i.e., \( d_c = -\ln(\xi) / \sigma'_t \)

for a particle in material \( i \). The distance to cell boundary, \( d_b \), is computed in the standard fashion. If the material interface crossing event is selected, the Monte Carlo particle is moved to the material interface location and the material identifier changed to the opposite material. If the collision event is selected, the particle is maintained in the same material following the collision. If the cell boundary crossing event is selected, the Monte Carlo particle is maintained in the same material to preserve the material previously sampled. The Monte Carlo LP algorithm resamples the distance to material interface on each particle track.

The Monte Carlo LP and LRP Monte Carlo algorithms differ in how they treat the distance to material interface values. The LP algorithm resamples a new distance to material interface in the direction of particle travel, \( d_i \), after every event—collision, material interface crossing, and cell boundary crossing. As a result, a particle encounters a different material realization following a collision, which is nonphysical. We therefore expect the Monte Carlo LP algorithm to be least accurate in materials with significant amounts of scattering and optically-thick mean chord lengths. In contrast, the LRP algorithm samples distance to material interface values in the forward and backward directions of particle travel, \( d_f^+ \) and \( d_f^- \), respectively, for each source particle. When a particle is moved, \( d_f^+ \) and \( d_f^- \) are decremented and incremented, respectively, by the distance moved. Following a collision, the distance to material interface values are either maintained as-is or switched to account for backscattering [4, 5]. In multiple dimensions, we perform this operation probabilistically based on the cosine of the angle between the incoming and outgoing particles, \( \mu \). The distance to material interface values are switched with probability \( P_{\text{switch}}(\mu) = \frac{1}{2} (1 - \mu) \), i.e., if \( \mu < 2\xi - 1 \), where \( \xi \) is a random number. This simple linear probabilistic model has the correct behavior in the forward- and back-scattering limits. In addition, the model preserves the average deflection cosine of the scattering, thereby obtaining the correct diffusion coefficient for all scattering laws. This probabilistic model usually maintains the distance to material interface values for forward-scattered particles and usually switches the values for back-scattered particles, with the
probability of switching increasing linearly as the particle is increasingly back-scattered. If $d^*_i$ is the minimum distance of events, the particle is moved to the material interface, the material identifier is switched, a new $d^*_i$ value is sampled, and $d^*_i$ is set to zero. In the Monte Carlo LRP algorithm, a particle can move, undergo collisions, and cross cell boundaries within one material and encounter the same local material realization, which is physically more realistic than the LP algorithm. As a result, we expect the Monte Carlo LRP algorithm to be more accurate than the LP algorithm. The LRP algorithm remains approximate if a particle reenters the same material at the same location within one history, as the sampled material realization will be different upon reentry.

**NUMERICAL RESULTS**

We implemented the Monte Carlo LP and LRP algorithms in an experimental version of the LLNL Kull implicit Monte Carlo (IMC) thermal photon transport package [6, 7, 13]. To solve the linear transport problems under investigation in this work with the IMC implementation, we used a large specific heat capacity to decouple the transport from the material. We performed the Monte Carlo AM, LP, and LRP simulations with $10^8$ Monte Carlo particles per time step, a spatial grid of $(10^3 \times 10^3 \times 10^3)$ zones, and 100 time steps of $5 \times 10^{-6}$ s. The AM results were computed using the LP algorithm with the same atomic-mixed cross sections in both materials. We compare the Monte Carlo AM, LP, and LRP results against the benchmark transport results from Ref. [10]. The cumulative ensemble-averaged reflection and transmission values from the simulations are shown in Tables II and III, respectively. We also show the relative error in a given value computed as $E_V = (V_{\text{approximate}} - V_{\text{benchmark}})/V_{\text{benchmark}}$. Finally, we have also computed three overall measures of accuracy: the root-mean-square of the error values along with the mean and maximum of the absolute value of the error values.

The AM approximation produces significant errors in both the reflection and transmission compared to the benchmark values for this set of stochastic medium transport problems, with the error in the transmission being generally larger. The AM approximation severely underpredicts the transmission. Pomraning [1] has argued that the atomic mix approximation always underestimates the transmission through a source-free random mixture, and our numerical results support that claim.

For the reflection, the RMS and mean error for the LP algorithm is 13% and 10%, respectively, with a maximum error of 26% for case 3b. The LP approximation reduces the error in the reflection by a factor of five compared to the AM approximation. The RMS and mean error for the LRP algorithm is 5% and 4%, respectively, with a maximum error of 10% for case 2b. The LRP algorithm therefore generally reduces the error in the reflection by a factor of two to three compared to the LP approximation. The LRP reflection values are more accurate than the LP values except for case 1b.

For the transmission, the RMS and mean error for the LP algorithm is 10% and 8%, respectively, with a maximum error of 18% for case 3a. The LP approximation reduces the error in the transmission by approximately a factor of ten compared to the AM approximation. The RMS and mean error for the LRP algorithm is 8% and 7%, respectively, with a maximum error of 12% for case 3a. The LRP algorithm therefore generally reduces the error in the transmission compared to the LP approximation by approximately 10-20%. The LRP transmission values are more accurate than the LP values except for cases 1b, 2b, and 3c.

**CONCLUSIONS**

We have compared the accuracy of 3D Monte Carlo AM, LP, and LRP transport algorithms for a suite of 3D binary stochastic medium benchmark problems [10] characterized by Markovian material statistics. The LP approximation is significantly more accurate than the AM approximation for these problems by a factor of five to ten. The LRP algorithm is more accurate overall than the LP approximation by a factor of two to three for reflection and 10-20% for transmission. We conclude that the LRP algorithm is generally an improvement over the LP algorithm for both 1D and 3D simulations.

In future work, we would like to investigate the properties of alternative probabilistic models for switching the forward and backward distance to material interface values in the LRP algorithm.

**ACKNOWLEDGMENTS**

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**REFERENCES**

3. M. L. ADAMS, E. W. LARSEN, and G. C. POMRANING, “Benchmark Results for Particle Transport in a...
TABLE II: Linear Transport Benchmark Suite Reflection Results

<table>
<thead>
<tr>
<th>Case</th>
<th>Benchmark [10]</th>
<th>AM</th>
<th>LP</th>
<th>LRP</th>
<th>Relative Error E_R</th>
<th>AM</th>
<th>LP</th>
<th>LRP</th>
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<tr>
<td>1</td>
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<td>0.4065</td>
<td>0.49533</td>
<td>0.40159</td>
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<td>0.390</td>
<td>-0.195</td>
<td>-0.002</td>
</tr>
</tbody>
</table>

RMS E_R
mean |ER|: 0.630, 0.127, 0.053
max |ER|: 1.221, 0.256, 0.096

TABLE III: Linear Transport Benchmark Suite Transmission Results

<table>
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<tr>
<th>Case</th>
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<th>AM</th>
<th>LP</th>
<th>LRP</th>
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<th>LP</th>
<th>LRP</th>
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RMS E_T
mean |ET|: 0.894, 0.096, 0.078
max |ET|: 1.000, 0.178, 0.122