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P. S. Brantley

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Benchmark Investigation of a 3D Monte Carlo Levermore-Pomraning Algorithm for Binary Stochastic Media

Patrick S. Brantley

Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, CA 94551
brantley1@llnl.gov

INTRODUCTION

In a stochastic medium, the material properties at a given spatial location are known only statistically [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]. Zimmerman and Adams [3] proposed a Monte Carlo algorithm that solves the LP equations, and this algorithm has been demonstrated using one-dimensional planar geometry benchmark studies to generally be more accurate than the atomic mix approximation [3, 4].

Brantley and Martos [5] generated using the Mercury Monte Carlo particle transport code [6] three-dimensional binary stochastic medium benchmark results for a particle transport problem with varying spherical inclusion mean chord lengths and three different radius distributions. That work 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 representative of turbulent media, for example.

In this work, we extend previous one-dimensional studies [3, 4] by investigating the accuracy of a multi-dimensional Monte Carlo Levermore-Pomraning algorithm for stochastic medium problems in which the shape of the inclusions is not explicitly known and the size of the inclusions is characterized only by a mean chord length. To accomplish this research, we implemented in Mercury a multi-dimensional extension of the one-dimensional Levermore-Pomraning binary stochastic medium algorithm [3, 4]. Different than related Monte Carlo chord length sampling work [7, 8] aimed at high temperature gas-cooled reactor applications in which the shape of the inclusions are known to be spherical TRISO fuel particles, we do not explicitly treat the inclusions as spheres in our Monte Carlo LP algorithm. In addition to being significantly simpler to implement, this approach is more appropriate for modeling transport through stochastic media in which the shape of the inclusions is not explicitly known. We investigate the accuracy of this multi-dimensional Monte Carlo LP algorithm using the spherical inclusion benchmark results of Ref. [5].

BINARY STOCHASTIC MEDIUM PROBLEM SUITE

We consider 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 ∂D :

$$\begin{aligned} \underline{\Omega} \cdot \underline{\nabla} \psi(\underline{x}, \underline{\Omega}) + \sigma_t(\underline{x}) \psi(\underline{x}, \underline{\Omega}) &= \\ &= \frac{\sigma_s(\underline{x})}{4\pi} \int_{4\pi} \psi(\underline{x}, \underline{\Omega}') d^2\Omega' \quad , \quad (1a) \end{aligned}$$

$$\psi(x, y, z = 0, \underline{\Omega}) = \frac{1}{2\pi} \quad , \quad 0 \leq x, y \leq L \quad , \quad \underline{\Omega} \cdot \underline{n} < 0 \quad , \quad (1b)$$

$$\psi(x, y, z = L, \underline{\Omega}) = 0 \quad , \quad 0 \leq x, y \leq L \quad , \quad \underline{\Omega} \cdot \underline{n} < 0 \quad . \quad (1c)$$

Here we have used standard neutronics notation [9]: ψ is the angular flux of particles [#/cm²-s-steradian] at a position $\underline{x} = (x, y, z)$ traveling in direction $\underline{\Omega}$; $\sigma_t(\underline{x})$ is the macroscopic total cross section [cm⁻¹] at position \underline{x} ; and $\sigma_s(\underline{x})$ is the macroscopic scattering cross section [cm⁻¹] at position \underline{x} . An isotropic angular flux with unity incoming current is incident on the left edge of the domain at $z = 0$, where \underline{n} is the unit outer normal to ∂D at a position \underline{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 transport problem is depicted schematically in Fig. 1. To generate benchmark results, we assume that the binary stochastic medium is composed of optically thick spherical inclusions with uniform material properties distributed in an optically thin background matrix material also with uniform material properties. The benchmark ensemble-averaged fiducial quantities of interest are the reflection and transmission rates as well as the absorption rates in the sphere and background matrix materials.

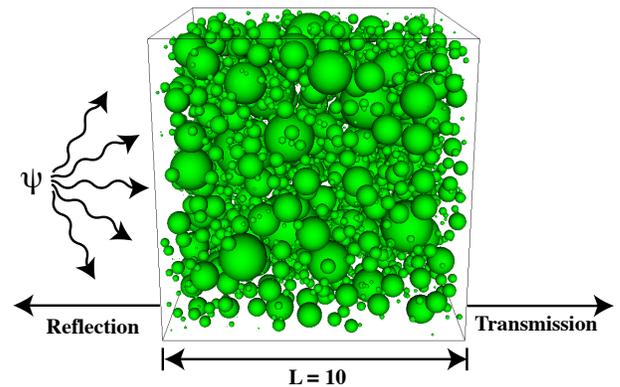


Fig. 1: Transport problem configuration.

We investigate a suite of binary stochastic medium transport problems characterized by the material parameters given in Table I [5]. Here material zero is the optically thin background matrix material, material one is the optically

thick inclusion material, and Λ_i is the mean chord length for material i . Both materials are assumed to have a scattering ratio of $c = \sigma_s/\sigma_t = 0.9$. These material parameters are variations of parameters originally used by Adams et al. [10] in the generation of one-dimensional benchmark transport solutions and provide a connection with related one-dimensional work [4].

The different case numbers in our benchmark suite represent variations of the spherical inclusion mean chord length. The mean chord length for any non-reentrant body is given by $\Lambda = 4V/A$, where V is the volume of the body and A is the surface area of the body. For a sphere of radius r , $\Lambda_{sphere} = 4r/3$. Different distributions of sphere radii characterized by a mean radius R will have different mean chord length values. The benchmark results against which we compare in this work were generated using an exponential sphere radius distribution [5]. The radius probability distribution function $p(r)$ for an exponential distribution along with the relationship between the sphere mean chord length Λ_1 and the sphere mean radius R are given by [11]

$$p(r) = \frac{1}{R} \exp\left(-\frac{r}{R}\right), \quad 0 \leq r \leq \frac{L}{6}, \quad R = \frac{1}{4}\Lambda_1. \quad (2)$$

The benchmark results were generated by sampling 100 independent material realizations for each sphere mean chord length case and each sphere volume fraction value. For the exponential radius distribution, we heuristically limited the maximum sampled sphere radius to be 1/6 of the domain edge length L to avoid problems placing multiple large spheres in the problem domain. For each sphere mean chord length case (1, 2, and 3), six different sphere volume fractions f_1 (0.05, 0.10, 0.15, 0.20, 0.25, and 0.30) were considered, where the sphere volume fraction f_1 is defined as the total volume of all spherical inclusions divided by the volume of the problem domain. If the sphere volume fraction f_1 and the sphere mean chord length Λ_1 are known, the mean chord length in the background matrix material can be computed for an infinite medium (ignoring boundary effects) as [1, 11]

$$\Lambda_0 = (1/f_1 - 1)\Lambda_1. \quad (3)$$

Each Monte Carlo simulation for an independent material realization used 2×10^6 particle histories, and the resulting standard deviation of the ensemble-averaged mean for each tally considered was computed to be less than 2% for all cases. Consistent with previous one-dimensional work [4, 10], we assume a domain size of $L = 10$.

MONTE CARLO LEVERMORE-POMRANING ALGORITHM

A detailed description of the Monte Carlo Levermore-Pomraning algorithm for one-dimensional planar geometries is given in Ref. [4]. The extension to multidimensional geometries is relatively straightforward.

Much of the standard Monte Carlo particle transport algorithm using the atomic 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 a 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 , λ_i , follow an exponential distribution given by

$$f_i(\lambda_i) = \frac{1}{\Lambda_i} \exp\left(-\frac{\lambda_i}{\Lambda_i}\right), \quad (4)$$

where Λ_i is the mean chord length for material i . (Olson et al. [11] demonstrate that the chord lengths in the background matrix are approximately exponential for the case of non-overlapping spherical inclusions when the sphere volume fraction is less than 10%.) 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 ξ is a random number. This sampling of a distance to material interface essentially 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 , is sampled using the macroscopic total cross section corresponding to the material in which the particle exists. The distance to cell boundary, d_b , is computed in the standard fashion. If the distance to material interface event is selected, the Monte Carlo particle is moved to the material interface location and the material identifier changed to the opposite material. Following a collision, the particle is maintained in the same material. The Monte Carlo LP algorithm resamples the distance to material interface on each particle track.

NUMERICAL RESULTS

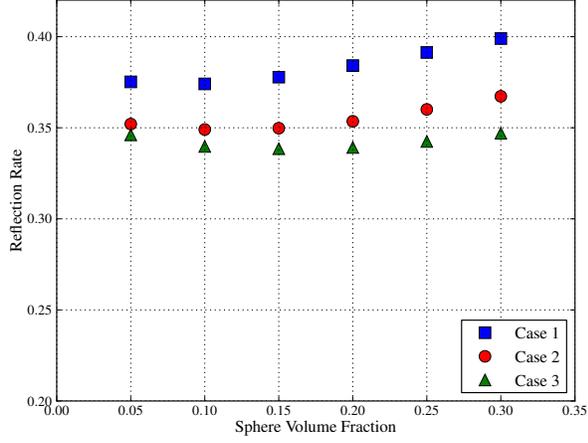
As an initial test of our Monte Carlo LP implementation, we simulated the binary stochastic medium particle transport benchmark suite of Adams et al. [10]. This one-dimensional planar geometry benchmark suite consists of three material mean chord length values and three material scattering ratio values (nine total combinations). For the nine cases simulated with a domain width of $L = 10$ cm and 10^9 Monte Carlo particles, the ensemble-averaged reflection and transmission values from the present Monte Carlo LP simulations agree with previous Monte Carlo LP results [4] to four or five decimal places (typically to within two standard deviations, where the maximum relative standard deviation is 0.09%). These Monte Carlo LP results also agree with the deterministic LP results in Ref. [10]. As an additional check of our implementation, we verified for one of the cases in our present work that the Monte Carlo LP results correctly limit to the atomic mix results in the limit of small sphere mean chord length.

We simulated the binary stochastic medium benchmark problem with Monte Carlo using both the AM approxima-

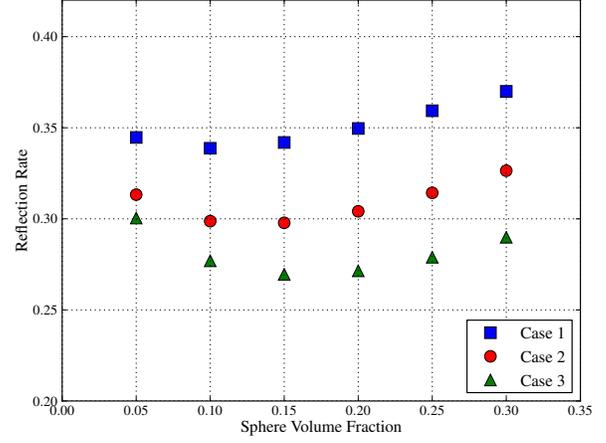
TABLE I: Material parameters for stochastic medium transport problems

Case	σ_t^0	Λ_0^*	$\sigma_t^0 \Lambda_0$	σ_t^1	Λ_1	$\sigma_t^1 \Lambda_1$	c
1		99/40	0.25		11/40	2.5	0.9
2	10/99	99/20	0.5	100/11	11/20	5.0	
3		99/10	1.0		11/10	10.0	

* For 10% sphere volume fraction; see Eq. (3).

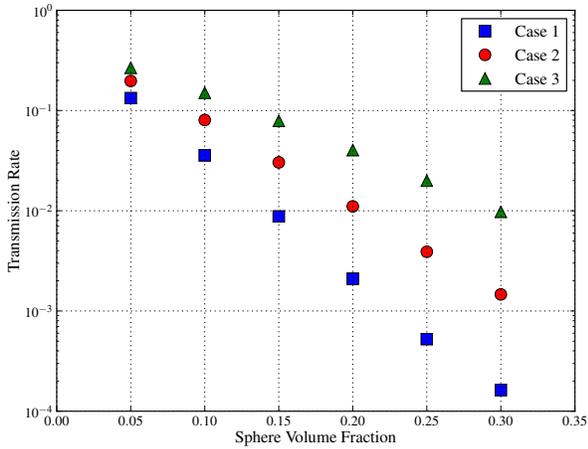


(a) Benchmark

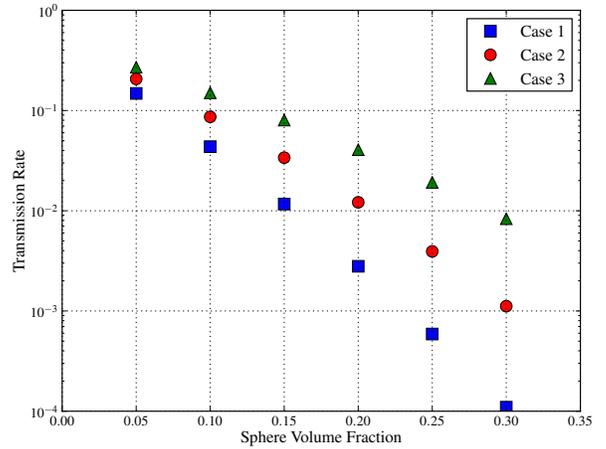


(b) LP approximation

Fig. 2: Reflection rate



(a) Benchmark



(b) LP approximation

Fig. 3: Transmission rate

tion and the LP approximation. We compare the reflection and transmission rates computed using these algorithms with the benchmark results [5]. The AM approximation produces identical results for Cases 1, 2, and 3, because the homogenized cross sections depend only on the material cross sections and volume fractions and are independent of the spherical inclusion mean chord length. Within a single material property case, the different material volume fractions produce different results when using the AM approxi-

mation. The benchmark and LP reflection and transmission rates are shown in Figs. 2 and 3, respectively. Our simulations used 10^8 Monte Carlo particles, producing typical relative standard deviations of a fraction of 1%. However, the AM transmission rate relative standard deviations were approximately 2%, 5%, and 19% for the three largest sphere volume fractions.

The AM approximation produces reflection rate values of approximately 0.48 for all sphere volume fractions,

overpredicting the reflection rate by approximately 20-41% compared to the benchmark result. The AM approximation severely underpredicts the transmission rate by approximately one order of magnitude for smaller sphere volume fractions and increasing to three orders of magnitude low for larger sphere volume fractions. 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.

Comparing Figs. 2(a) and 2(b), the LP approximation underpredicts the reflection rate compared to the benchmark result by approximately 7-20%, with Case 1 (smallest inclusion mean chord length) the most accurate and Case 3 (largest inclusion mean chord length) the least accurate. The LP approximation qualitatively captures the trends evident in the reflection rate as a function of the sphere volume fraction. Comparing Figs. 3(a) and 3(b), the LP approximation generally overpredicts the transmission rate compared to the benchmark result except for the highest sphere volume fractions. The transmission rate discrepancies observed for Case 1 range from -33% to +33%, for Case 2 from -25% to +11%, and for Case 3 from -15% to +2%. For the stochastic medium problems examined, 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. Although not shown due to space limitations, we find that the LP approximation overpredicts the spherical inclusion absorption rate by 4-20% and underpredicts the matrix absorption rate by 1-27%. In general, the magnitude of these discrepancies is similar to those observed in 1D studies with 10 cm spatial domains [4].

CONCLUSIONS

We have examined the accuracy of a multi-dimensional Monte Carlo Levermore-Pomraning algorithm for stochastic medium transport problems in which the shape of inclusions may not be known and the size of inclusions is characterized by a mean chord length value. As an initial investigation of the accuracy of this method, we modeled a suite of benchmark stochastic medium transport problems in which the inclusion variation was restricted to spherical inclusions with radii described by an exponential distribution. We found that the LP approximation produced consistently more accurate results than the AM approximation. The discrepancies between the LP approximation and the benchmark results were up to 20% for the reflection rate and up to 33% for the transmission rate, however. Given these discrepancies, the development of stochastic medium algorithms that are more accurate than the LP approximation would appear to be a fruitful area of future research.

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