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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. The AM approximation is conceptually simple and computationally efficient but may not be accurate enough for a given application. A common deterministic model developed specifically for solving linear 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 is equivalent to the LP approximation.

Thermal radiative transfer problems are characterized by a radiation field tightly coupled to a participating material energy field. Radiative transfer through a stochastic medium can occur, for example, in inertial confinement fusion targets in which hydrodynamic instabilities at material interfaces can produce a turbulent (stochastic) medium. Miller [4] and Miller et al. [5] first investigated the solution of binary stochastic medium radiative transfer problems with a participating medium. They generated benchmark ensemble-averaged results for a particular binary stochastic medium radiative transfer problem and compared the accuracy of the atomic mix approximation, an adaptation of the standard deterministic LP model to radiative transfer with participating media, and an adaptation of a deterministic model that attempts to incorporate the effects of scattering in the statistical coupling terms arising in the LP model. For the binary stochastic medium benchmark problem examined, the AM approximation generally under-predicts transmission of radiation and the LP approximation generally over-predicts transmission.

The implicit Monte Carlo (IMC) algorithm [6] has become the standard Monte Carlo algorithm for modeling time-dependent thermal radiative transfer problems. In this work, we describe the extensions to the IMC algorithm required to incorporate the Monte Carlo LP algorithm originally proposed by Zimmerman and Adams [3] for the solution of linear particle transport problems in binary stochastic media. We demonstrate numerically that the proposed IMC algorithm reproduces the deterministic LP model results obtained by Miller [4] and Miller et al. [5].

LEVERMORE-POMRANING IMC ALGORITHM

We consider thermal photon transport in a binary stochastic medium described by temporally-stationary and spatially-homogeneous isotropic statistics. In the absence of physical scattering and external sources, the grey implicit Monte Carlo equations [6] for material i of a binary stochastic medium including the Levermore-Pomraning closure for the coupling of materials [2, 5] are given by:

$$\frac{1}{c}\frac{\partial I_i}{\partial t} + \underline{\Omega}\cdot\underline{\nabla} I_i + \sigma_i^n I_i = \frac{1}{4\pi}\sigma_i^n\left(1-f_i^n\right)\int_{4\pi} I_i d^2\Omega' + \frac{1}{4\pi}\sigma_i^n f_i^n c u_{r,i}^n + \frac{1}{\Lambda_j} I_j - \frac{1}{\Lambda_i} I_i \ , \tag{1a}$$

$$u_{m,i}^{n+1} = u_{m,i}^n + \sigma_i^n f_i^n \int_{t^n}^{t^{n+1}}\int_{4\pi} I_i d^2\Omega dt - \sigma_i^n f_i^n \Delta t^n c u_{r,i}^n \ . \tag{1b}$$

Here $\underline{\Omega}$ is the direction of photon travel, t is the time, c is the speed of light, and σ_i is the absorption opacity for material i. $I_i\left(\underline{r},\underline{\Omega},t\right)$ is the intensity of radiation at position $\underline{r}$ traveling in direction $\underline{\Omega}$ at time t conditioned on material i being present at position $\underline{r}$ and time t. $u_{r,i} = aT_i^4$ is the equilibrium radiation energy density in material i, where a is the radiation energy density constant and T_i is the temperature in material i, and $u_{m,i}$ is the material energy density in material i. A superscript n denotes a quantity evaluated at the beginning of the time step. The quantity $f_i^n = \frac{1}{1+\beta_i^n c\sigma_i^n\Delta t^n}$, where $\beta_i = \frac{\partial u_{r,i}}{\partial u_{m,i}}$, is the "Fleck factor" in material i that serves to model a portion of the absorption and subsequent reemission of photons within a time step Δt^n as effective isotropic scattering. The last two terms on the right side of Eq. (1a) arise from the Levermore-Pomraning model for stochastic medium transport. The term $\frac{1}{\Lambda_i} I_i$ can be interpreted as the rate per unit volume at which photons at position $\underline{r}$ and moving in direction $\underline{\Omega}$ exit material i and enter material j; $\frac{1}{\Lambda_i}$ can then be interpreted as a probability per unit path length that a particle in material i enters material j. The other coupling term has an analogous interpretation and represents a source of particles entering material i from material j. Eq. (1b) is a material energy balance equation for material i.

Much of the standard implicit Monte Carlo algorithm using the atomic mix approximation is unaltered by the introduction of algorithms to model radiative transfer through

a stochastic medium. A Monte Carlo photon must maintain an additional identifier describing the material in which the photon is currently located. This material identifier must be appropriately sampled (in proportion to the material probability) when a photon is created from a source or enters the problem via an external boundary. The IMC equations are typically solved using a spatial mesh with Monte Carlo photons advanced over time steps. In addition to the standard distance to collision, distance to zone boundary, and distance to census values that must be sampled or computed [6], a new event, the distance to material interface, d_{int}, is sampled from the appropriate distribution characterizing the chord lengths in the material. For Markovian statistics, the chord lengths λ_i are given by the exponential distribution

$$m_i(\lambda_i) = \frac{1}{\Lambda_i} \exp\left(-\frac{\lambda_i}{\Lambda_i}\right) \ , \tag{2}$$

where Λ_i is the mean chord length in material i. If the distance to material interface event is selected, the Monte Carlo photon is moved to the material interface location and the material identifier changed to the opposite material. An important aspect of the algorithm in a stochastic medium is to keep the Monte Carlo photon in the same material when a zone boundary is crossed to preserve the sampled local material realization. (This portion of the algorithm must be modified if spatially inhomogeneous material statistics are present.) In addition, particles retrieved from census at the beginning of the time step should remain in the same material in which they were placed into census at the end of the previous time step to avoid a dependence of the results on the time step size. (This portion of the algorithm must be modified if temporally non-stationary material statistics are present.) Finally, a material energy balance equation for each material is required.

NUMERICAL RESULTS

We implemented the Levermore-Pomraning IMC algorithm in an experimental version of the LLNL Kull IMC package [7]. This IMC package already possessed multiple material infrastructure that aided the implementation of the modifications required to enable the LP algorithm. The implementation of the stochastic medium transport algorithm is general (multiple spatial dimensions, multigroup opacities, parallelism via domain decomposition and replication), although testing of the capability to this point has focused on one-dimensional planar geometry grey radiative transfer problems.

As an initial test of the capability, we simulated the binary stochastic medium linear particle transport benchmark suite of Adams et al. [8]. This time-independent one-dimensional planar geometry benchmark suite consists of three spatial domain widths, three material mean chord length combinations, and three material scattering ratio combinations (27 total cases). We used a large specific heat capacity to decouple the transport from the material for this linear benchmark suite. For the 27 cases simulated, the ensemble-averaged reflection and transmission values from our IMC simulations agree with previous LP Monte Carlo results [9] to typically three to four digits (significantly better than 1%). These Monte Carlo LP results also agree with the deterministic LP results in Ref. [8].

We investigate in more detail here the binary stochastic medium benchmark radiative transfer suite of Miller [4] and Miller et al. [5]. This one-dimensional planar geometry benchmark suite consists of a strongly absorbing material 1 (σ_1 = 1000 cm^{-1}) with smaller mean chord length mixed with a more weakly absorbing material 2 (σ_2 = 5 cm^{-1}) with larger mean chord length. The problem spatial domain is given by $0 \leq z \leq L$ = 0.15 cm. The materials are distributed according to Markovian statistics (exponentially) with the mean chord lengths given in Table 1. (We note that the mean chord length values are listed incorrectly in Ref. [5]; the correct values given in Ref. [4] are one order of magnitude smaller.) For the specified mean chord lengths, the probability of material i being present, $p_i = \frac{\Lambda_i}{\Lambda_1+\Lambda_2}$, is constant for all mean chord length cases. As a result, the atomic mix approximation result is the same for all cases. The initial temperature of the materials is T_{init} = 30 eV, and a cosine-distributed source of radiation at 300 eV is present at $z = 0$. A special form of the specific heat capacity is assumed, $C_{v,i} = \frac{4a}{\rho_i} T_i^3$, where ρ_i is the mass density of material i, which results in a linearization of the material energy balance equation. We simulated this problem using the IMC package with the LP model using 3×10^6 Monte Carlo photons per time step, one thousand uniformly-spaced zones, and an initial time step of 10^{-15} s with a maximum time step of 10^{-12} s.

Table 1: Benchmark Problem Parameters

Problem	Λ_1	Λ_2
	[cm]	[cm]
A	5.0e-3	5.0e-1
B	5.0e-4	5.0e-2
C	5.0e-5	5.0e-3
D	5.0e-6	5.0e-4
E	Atomic Mix	

We plot in Fig. 1 the ensemble-averaged temperature energy density at the outgoing edge ($z = L$) of the spatial domain scaled by the initial temperature for each of the cases simulated. The ensemble-averaged temperature energy density is computed from the material temperatures using [5]

$$\left\langle aT^4 \right\rangle = p_0 a T_0^4 + p_1 a T_1^4 \ , \tag{3}$$

where p_i is the probability of material i being present, as described above. The material temperature in the simulation code is zone-centered, so we plot the temperature in

the zone closest to the boundary to represent the value at $z = L$. We plot in Fig. 2 the ensemble-averaged transmission at the outgoing edge ($z = L$) of the spatial domain scaled by the initial temperature, where the transmission is given by

$$\langle Trans \rangle = \left\langle \int_0^1 \mu I\left(L, \mu, t\right) d\mu \right\rangle \quad . \tag{4}$$

The ensemble-averaged transmission is numerically computed by tallying the energy weight of Monte Carlo photons escaping the domain at $z = L$. By inspection, we observe that the LP IMC results for the exiting ensemble-averaged temperature and transmission agree with the deterministic LP results in Refs. [4] and [5]. (The numerical data from Refs. [4] and [5] is no longer available and has not yet been reproduced.) We also observe that the material temperature at $z = L$ and the transmission computed using the LP IMC algorithm is higher for cases with larger mean chord lengths and limits in the steady state to the atomic mix result as the mean chord lengths decrease. For the smallest mean chord length case, the discrepancy in the transient temperature and transmission profiles between the LP model (curve D) and the AM approximation (curve E) was also observed in Refs. [4] and [5]. This discrepancy was subsequently investigated using asymptotic analysis in Ref. [10]. Though not examined here, the LP approximation is shown in Refs. [4] and [5] to be more accurate than the atomic mix approximation for larger mean chord lengths and is more accurate in the small mean chord length limit during the transient phase.

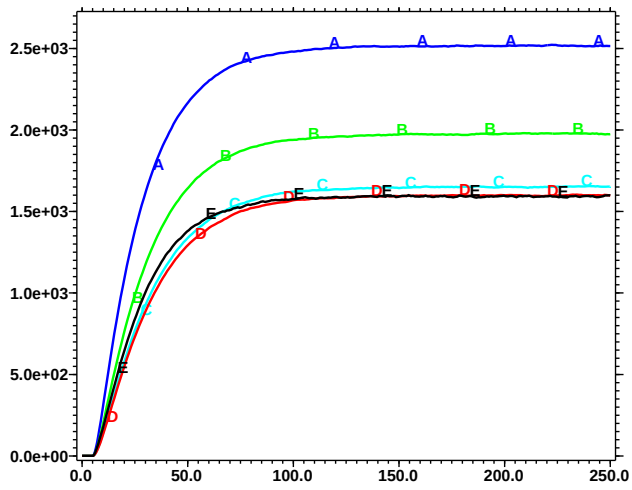

Figure 1: $\left\langle aT^4 \right\rangle / aT_{init}^4$ at $z = L$ versus time ($\times 10^{-12}$ s)

CONCLUSIONS

We described the modifications to the standard implicit Monte Carlo algorithm for thermal radiative transfer necessary to implement the Levermore-Pomraning approximation for binary stochastic media. Simulations

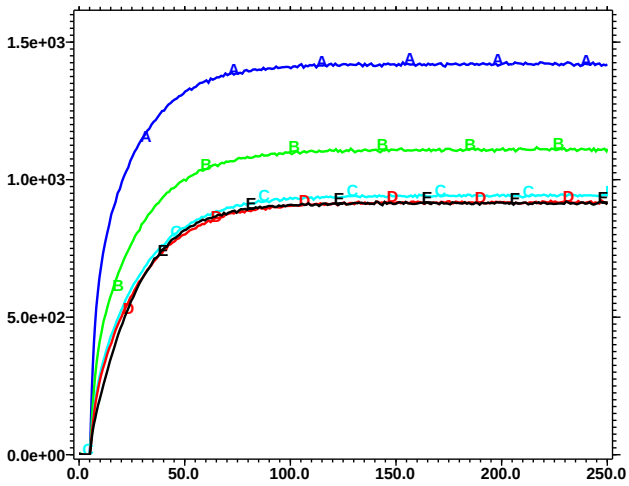

Figure 2: $\langle Trans \rangle / caT_{init}^4$ at $z = L$ versus time ($\times 10^{-12}$ s)

of a radiative transfer benchmark suite using the modified IMC algorithm numerically demonstrate agreement with deterministic Levermore-Pomraning solutions. In future work, we plan to investigate additional algorithms with the aim of improving on the accuracy of the Levermore-Pomraning approximation for radiative transfer in binary stochastic media.

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