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A Hybrid Monte Carlo-Deterministic Method for Global Binary Stochastic Medium Transport Problems

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INTRODUCTION

Global deep-penetration transport problems are difficult to solve using traditional Monte Carlo techniques. In these problems, the scalar flux distribution is desired at all points in the spatial domain (global nature), and the scalar flux typically drops by several orders of magnitude across the problem (deep-penetration nature). As a result, few particle histories may reach certain regions of the domain, producing a relatively large variance in tallies in those regions. Implicit capture (also known as survival biasing or absorption suppression) [1] can be used to increase the efficiency of the Monte Carlo transport algorithm to some degree. A hybrid Monte Carlo-deterministic technique has previously been developed by Cooper and Larsen [2] to reduce variance in global problems by distributing particles more evenly throughout the spatial domain. This hybrid method uses an approximate deterministic estimate of the forward scalar flux distribution to automatically generate weight windows [3] for the Monte Carlo transport simulation, avoiding the necessity for the code user to specify the weight window parameters.

In a binary stochastic medium, the material properties at a given spatial location are known only statistically [4]. The most common approach to solving particle transport problems involving binary stochastic media is to use the atomic mix (AM) approximation [4] in which the transport problem is solved using ensemble-averaged material properties. The most ubiquitous deterministic model developed specifically for solving binary stochastic media transport problems is the Levermore-Pomraning (L-P) model [4, 5]. Zimmerman and Adams [6] proposed a Monte Carlo algorithm (Algorithm A) that solves the Levermore-Pomraning equations and another Monte Carlo algorithm (Algorithm B) that is more accurate as a result of improved local material realization modeling [6, 7]. Recent benchmark studies [7] have shown that Algorithm B is often significantly more accurate than Algorithm A (and therefore the L-P model) for deep penetration problems such as examined in this paper.

In this research, we investigate the application of a variant of the hybrid Monte Carlo-deterministic method proposed by Cooper and Larsen to global deep penetration problems involving binary stochastic media. To our knowledge, hybrid Monte Carlo-deterministic methods have not previously been applied to problems involving a stochastic medium. We investigate two approaches for computing the approximate deterministic estimate of the forward scalar flux distribution used to automatically generate the weight windows. The first approach uses the atomic mix approximation to the binary stochastic medium transport problem and a low-order discrete ordinates angular approximation. The second approach uses the Levermore-Pomraning model for the binary stochastic medium transport problem and a low-order discrete ordinates angular approximation. In both cases, we use Monte Carlo Algorithm B with weight windows automatically generated from the approximate forward scalar flux distribution to obtain the solution of the transport problem.

PROPOSED HYBRID ALGORITHM

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

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

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

$$\psi(0,\mu) = 2 \ , \ \mu > 0 \ , \tag{1b}$$

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

Eqs. (1) are written in standard neutronics notation [1]. The boundary conditions given by Eqs. (1b) and (1c) are non-stochastic and represent an isotropic incident angular flux with a unity partial incoming current at $x = 0$ and a vacuum boundary at $x = L$. 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. Because the macroscopic cross sections are random variables, the angular flux is also a random variable. The distribution of material slab widths in the planar medium is assumed to be described by spatially homogeneous Markovian statistics [4].

We implemented deterministic discrete ordinates codes that solve the atomic mix [4] and the Levermore-Pomraning [4, 5] approximations to the binary stochastic medium transport problem given. These discrete ordinates codes use standard Gauss-Legendre quadrature sets and the diamond difference spatial discretization [1]. We also implemented a Monte Carlo code that solves the binary stochastic medium transport problem using Algorithm B proposed by Zimmerman and Adams [6]. The Monte Carlo code can use analog Monte Carlo techniques and also the implicit capture and weight windows variance reduction techniques. Because the flux of particles can be significantly different for the two materials at the same spatial location, we use material-dependent weight windows. The weight windows are applied at collisions and at both zone boundary and material interface crossings.

We use the approximate scalar flux distribution computed using the discrete ordinates code, either AM or L-P, with a low-order angular quadrature to automatically estimate the weight windows. The center, ceiling, and floor of the weight window in material i are computed using [2]

$$ww_i^{center}\left(x\right) = \frac{\phi_i\left(x\right)}{\max \phi_i\left(x\right)} \quad , \tag{2a}$$

$$ww_i^{ceiling}\left(x\right) = \rho \times ww_i^{center}\left(x\right) \quad , \tag{2b}$$

$$ww_i^{floor}\left(x\right) = \frac{ww_i^{center}\left(x\right)}{\rho} \quad , \tag{2c}$$

where $\phi_i\left(x\right)$ is the material i scalar flux distribution and $\rho \geq 1$ is a scale factor. Using weight windows defined as in Eqs. (2) results in Monte Carlo particles distributed approximately uniformly across the problem domain [2]. When using the AM solution, the same flux is used to generate the weight windows in both materials, so the resulting weight windows are the same in both materials. Because the deterministic solution is computed on a finer spatial mesh than that used for the Monte Carlo weight windows, the deterministic solution is volume-averaged onto the coarser weight window spatial mesh.

NUMERICAL RESULTS

We consider a binary stochastic medium defined by $\sigma_t^0 = 10/99$, $\Lambda_0 = 99/100$, $\sigma_t^1 = 100/11$, and $\Lambda_1 = 11/100$ with a total slab width L = 25 cm. The scattering ratio, $c_i = \sigma_s^i/\sigma_t^i$, is the same in both materials, $c_0 = c_1 = 0.7$. Therefore, the stochastic medium consists of two materials with mean material slab widths of 0.1 and 1.0 mean free paths, respectively. The ensemble-averaged macroscopic total cross section is unity. This test problem specification is a binary stochastic medium variant of a test problem used by Becker, Wollaber, and Larsen [8] to investigate hybrid Monte Carlo-deterministic algorithms. For the deterministic L-P solution, we used the S_2 discrete ordinates approximation and uniform spatial zones with $\Delta x = 0.1$ cm (zones of approximately unity mean free path in material one). We generated the deterministic AM solution using the S_4 discrete ordinates approximation and uniform spatial zones with $\Delta x = 0.05$ cm. Deterministic AM results computed using the S_2 approximation were so inaccurate that the Monte Carlo solution was too inefficient to be practical. Larger zone sizes would most likely be sufficient for generating the approximate AM or L-P forward solution but would violate the positivity requirements of the diamond difference spatial discretization [1]. The Monte Carlo solutions were obtained using 10^7 histories, a weight window scale factor of $\rho = 4$, and uniform spatial zones with $\Delta x = 1.0$ cm. The Monte Carlo zone size is consistent with that used in similar studies by Becker et al. [8], also demonstrating the ability of the hybrid method to use disparate zone sizes in the deterministic and Monte Carlo algorithms.

We compare the results of the hybrid Monte Carlo-deterministic method using implicit capture and weight windows (WW) to the results obtained using implicit capture and a Russian roulette weight cutoff (IC). We evaluate the efficiency of the Monte Carlo methods using a material scalar flux distribution figure of merit (FOM) defined as

$$FOM_i\left(x\right) = \frac{1}{R_i^2\left(x\right) T_{cpu}} \quad , \tag{3}$$

where $R_i^2\left(x\right)$ is the relative standard deviation in the ensemble-averaged material i scalar flux distribution at a spatial location x, and T_{cpu} is the total CPU time required for the generation of the approximate deterministic solution (if required) and the Monte Carlo transport process. A high FOM value is desirable, as this indicates a small relative variance in the flux and/or a small CPU time.

The ensemble-averaged material scalar flux distributions computed for the test problem using the AM and the L-P models with the S_4 and S_2 angular approximations, respectively, and using Monte Carlo Algorithm B are plotted in Fig. 1. The L-P model demonstrates only reasonable agreement with the more accurate Monte Carlo results for this problem. The material scalar flux distributions and the leakage rate at $x = L$ computed using the L-P S_2 approximation exhibit relative differences with respect to the Monte Carlo of up to approximately 40%. The scalar flux distribution computed using the AM approximation is in error by a few orders of magnitude over much of the spatial domain. The inaccuracy of the AM approximation persists for higher discrete ordinates quadrature orders, i.e. the inaccuracy is a result of the AM approximation itself and not the angular quadrature order. The extreme inaccuracy of the AM approximation for this problem results in weight window values that produce an inefficient Monte Carlo calculation due to excessive particle splitting.

The material scalar flux distribution figure of merit values are plotted in Fig. 2 for the Monte Carlo simulations using implicit capture alone and for the simulations with weight windows automatically generated from the AM and L-P solutions. The FOM obtained using the hybrid Monte Carlo-deterministic method with weight windows computed from the approximate AM solution is larger than the IC FOM over a limited range of the spatial domain but is a few orders of magnitude lower over much of the domain. The FOM obtained using the hybrid method with weight windows computed from the approximate L-P solution is a few orders of magnitude larger than the IC FOM over much of the spatial domain. At $x = 25$, the hybrid method FOM is approximately three orders of magnitude larger than the IC FOM.

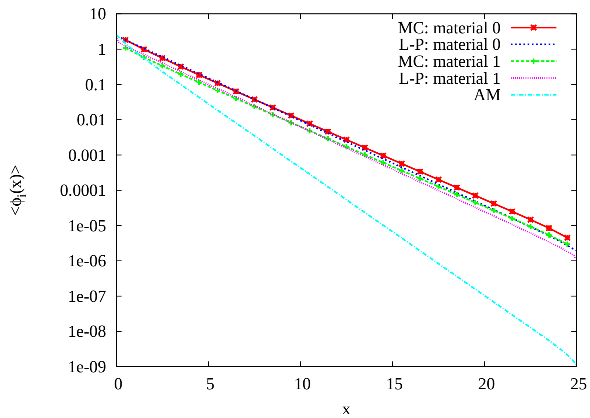

Figure 1: Scalar flux distributions

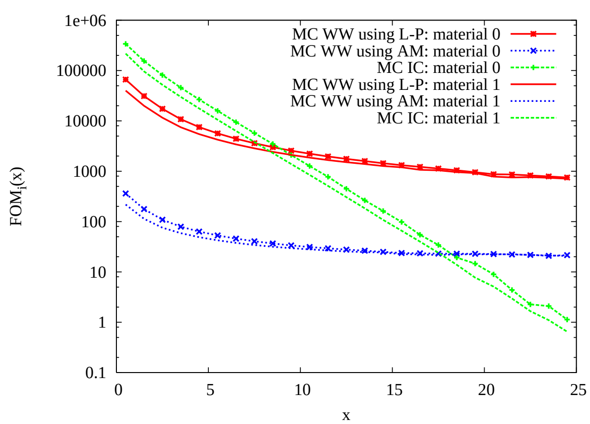

Figure 2: Scalar flux FOM values

CONCLUSIONS

We described a hybrid Monte Carlo-deterministic algorithm for automatically generating weight windows for global particle transport problems involving binary stochastic media. For the test problem investigated, the AM approximation is extremely inaccurate and produces an inefficient Monte Carlo result. The L-P model with an S_2 angular quadrature is only reasonably accurate for this problem, but the weight windows generated from the approximate L-P solutions produce significant efficiency improvements compared to the implicit capture results. These numerical results demonstrate that an approximate solution generated using the atomic mix approximation may not be adequate for use with the hybrid method, although this conclusion will most likely be problem-dependent. In general, using a more accurate approximate deterministic solution should be advantageous but must be weighed against the additional computational expense required to obtain the improved accuracy.

These preliminary numerical results demonstrate the potential of the hybrid method for global particle transport problems involving binary stochastic media. For some other combinations of stochastic material properties, the proposed hybrid method does not give significant improvements in the FOM compared to implicit capture, although the Monte Carlo particles are distributed more uniformly across the spatial domain. Further investigation is required to understand the fundamental cause of this behavior.

For the preliminary test problem examined in this paper, generally accurate results can be obtained using the L-P model. For more realistic stochastic medium transport problems in multiple dimensions and including energy dependence, other considerations such as improved energy resolution, improved geometric fidelity, or incorporation of relevant physics models may make the Monte Carlo method more attractive or even necessary. The basic concept of the proposed hybrid method should remain applicable to chord length sampling Monte Carlo methods that can be used to solve such problems. In that case, the approximate deterministic solution used to generate the weight windows could be obtained using either the atomic mix approximation if accurate enough or a multi-dimensional extension of the Levermore-Pomraning model [4]. The evaluation of the effectiveness of such a hybrid approach is beyond the scope of the present paper.

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