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Use of Woodcock Tracking to Enable Deferred Material Definition for Transport in Stochastic Media

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INTRODUCTION

Radiation transport in stochastic media is a challenging problem with a multitude of applications, and there has been a proliferating exigency to develop a method that is both accurate and efficient in producing computed quantities of interest for this type of problem. A matured method would be one that can be applied to multi-dimensional and multi-material geometries of arbitrary mixing types while producing accurate results efficiently. As a preliminary step in approaching this problem, in this work we investigate producing mean results and material-dependent flux profiles for radiation transport in one-dimensional, binary, Markovian-mixed media using a new method based on Woodcock tracking called Conditional Point Sampling (CoPS).

Many approximate methods have been developed as an alternative to the computationally expensive yet accurate benchmark method, which performs transport on a plethora of realizations generated using a brute-force implementation. The atomix mix (AM) approximation and the Levermore-Pomraning (LP) closure or its Monte Carlo equivalent, Chord Length Sampling (CLS) [1, 2], are the most well-known approximate methods. The AM approximation can be applied to all types of stochastic media because transport is performed on a geometry where the materials are homogenized. However, this approximate method generally lacks accuracy because of that homogenization. The LP closure is generally more accurate than the AM approximation for Markovian-mixed media. Its Monte Carlo equivalent, CLS, samples chord lengths of materials in real-time as the particle streams. However, it does not retain any memory of the material type after each interaction, introducing error in the mean results it produces.

Woodcock tracking [3, 4] is used to make real-time material assignments at potential collision sites in Conditional Point Sampling (CoPS). Because materials are sampled at points rather than on chords, material boundaries are not defined in the algorithm. Full memory of point-based material assignments is retained as materials are defined conditionally on previously defined points during the particle lifetime. Conditional probability functions are derived to have a close affinity to material-statistics correlation functions [5]. The fidelity of an imperfect conditional probability function dictates the accuracy of the method, as no bias error is introduced by the CoPS algorithm itself. For 1D, binary, Markovian-mixed media, we derive an approximate conditional probability function that defines the probability of sampling a new material type based on the material assignment of the nearest point. We believe that the information provided by the 2-point correlation functions used in material sciences is adequately assimilated in this derived 2-point conditional probability function. Using our derived 2-point conditional probability function in CoPS, we produce mean leakage results and material-dependent spatial flux distributions for the benchmark suite that was produced and expanded on in Ref. [1] and Ref. [2], respectively.

PROBLEM DESCRIPTION

We are interested in the stochastic radiation transport problem for one-dimensional, binary, Markovian-mixed media on a slab geometry with an isotropic boundary source at the left boundary and otherwise vacuum boundary conditions. Typically, to generate a realization for this type of problem, chord lengths of alternating material types are sampled beginning at the boundary [1, 2]. To perform transport on this type of media using CoPS, we derive our conditional probability function based on a less-common method of generating a realization introduced in Ref. [6]. This method places "pseudo-interfaces" within the domain using the Poisson-distribution of those pseudo-interfaces in Markovian-mixed media [7]. The correlation length of the material

$$\Lambda_c = \frac{\Lambda_\alpha \Lambda_\beta}{\Lambda_\alpha + \Lambda_\beta}, \tag{1}$$

is used to find the Poisson frequency of k pseudo-interfaces

$$f\left(k, \frac{r}{\Lambda_C}\right) = e^{-\frac{r}{\Lambda_C}} \left(\frac{\frac{r}{\Lambda_C}^k}{k!}\right), \tag{2}$$

where Λ_α and Λ_β are the average chord lengths in materials α and β [6], and $\frac{r}{\Lambda_C}$ is the average number of pseudo-interfaces per slab of length r. The number of pseudo-interfaces in a realization is calculated using Eq. (2), and they are randomly placed within the domain using a uniform distribution to define the boundaries of each cell. The material abundances are then used to sample the material in each cell. The abundance of material α for binary media made up of materials α and β is

$$P_\alpha = \frac{\Lambda_\alpha}{\Lambda_\alpha + \Lambda_\beta}. \tag{3}$$

CONDITIONAL POINT SAMPLING

The Conditional Point Sampling (CoPS) algorithm, the derivation for the two-point conditional probability function used in CoPS for binary, Markovian-mixed media, and discussion of how material-dependent collision flux tallies are taken are presented here. For different material-mixing types, a conditional probability function specific to that type must be approximated except in some special cases where a perfect conditional probability function may be derivable. Errors in results produced by CoPS are due to the approximations made in the derivation of those conditional probability functions, not the algorithm itself, which does not introduce any error and can be applied to any arbitrary mixing type.

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CoPS Algorithm

Conditional Point Sampling uses Woodcock tracking [3, 4] to stream particles to potential collision sites without having to define material locations or material boundaries. The CoPS algorithm begins by initializing a particle with a position x and direction μ. The first event is determined by taking the minimum of the distance to a potential collision and the distance to a crossed domain boundary. The distance to a potential collision is sampled using

$$d_c^* = -\frac{1}{\Sigma_t^*} log(\xi), \tag{4}$$

where Σ_t^* is the largest total cross section (aka, the majorant cross section) in the domain and ξ is a randomly generated number uniformly distributed between 0 and 1. The distance to boundary is

$$d_b = \begin{cases} \frac{x}{|\mu|}, & \mu < 0, \\ \frac{L-x}{|\mu|}, & \mu > 0, \end{cases} \tag{5}$$

where L is the slab length. If the minimum distance is the distance to boundary, the external boundary is crossed, and the particle is terminated. If the minimum distance is the distance to a potential collision site, the particle streams to that site, and we sample the material at that point conditionally on previously defined points. We then sample if the potential collision is accepted using a probability equal to the ratio of the true and majorant cross sections:

$$P_{col} = \frac{\Sigma_t}{\Sigma_t^*}. \tag{6}$$

We evaluate the collision if it is accepted. Otherwise, the particle continues to stream, and this algorithm repeats until it leaks or is absorbed.

2-Point Conditional Probability Function

To be true to the material properties of the materials being sampled as a particle streams, we sample new points conditionally based on points that have already been defined. Conditional probability functions are used to determine the probability of sampling material j at a potential collision site based on its distance away from the predefined points in the domain. For 2-point Conditional Point Sampling, we use just the nearest point at which material α or β can exist to approximate the 2-point conditional probability function. The probability of sampling material α is $\pi(\alpha|m, r)$, where m is the material type of the nearest point at a distance r away.

To derive this conditional probability function, we evaluate the permutations of having zero or at least one pseudo-interface using the Poisson frequency. For a scenario where there are no pseudo-interfaces between the point of interest and the nearest point, the material of the point of interest must be the same as the material at the nearest point. For a scenario where there exist pseudo-interfaces between the point of interest and the nearest point, the material abundance is used to sample the material type. The sum of these two products is given by Eqs. (7a) and (7b), where the material of the nearest point is defined as material α and material β, respectively:

$$\pi(\alpha|\alpha, r) = (1)f(k = 0, r) + (P_\alpha)f(k > 0, r), \tag{7a}$$

$$\pi(\alpha|\beta, r) = (0)f(k = 0, r) + (P_\alpha)f(k > 0, r). \tag{7b}$$

These reduce to

$$\pi(\alpha|\alpha, r) = 1 - \left(1 - P_\alpha\right)\left(1 - e^{-\frac{r}{\Lambda_c}}\right), \tag{8a}$$

$$\pi(\alpha|\beta, r) = P_\alpha\left(1 - e^{-\frac{r}{\Lambda_c}}\right). \tag{8b}$$

The probability of sampling material β for each scenerio is then

$$\pi(\beta|m, r) = 1 - \pi(\alpha|m, r). \tag{9}$$

Collision Tallies

Here, we present how collision tallies were taken to produce material-dependent spatial flux distributions. Traditionally, particle collisions in a cell are tallied and normalized over the cell size, total cross section, and total number of simulated particles [8]:

$$\phi_i = \frac{1}{\Delta x_i \Sigma_t} \frac{1}{N} \sum_n^N c_{n,i}, \tag{10}$$

where Δx_i is the size of cell i, Σ_t is the total cross section, N is the total number of simulated particles, and $c_{n,i}$ is the number of collisions tallied for history n in cell i. Equation (10) can be used to perform material-independent collision tallies.

Woodcock tracking can be used to conduct tallies at an increased collision rate by tallying at pseudo-collision sites to yield well-resolved flux distributions in geometries that have a minimal amount of true collisions (i.e. an optically thin portion of a slab). This generally improves the flux tally figure of merit (FOM) [3, 4]. In CoPS, we choose to tally all pseudo-collisions with a contributed weight of $\frac{\Sigma_t}{\Sigma_t^*}$, the probability of having a true collision:

$$\phi_i = \frac{1}{\Delta x_i \Sigma_t(x)} \frac{1}{N} \sum_n^N c_{n,i}^* \left(\frac{\Sigma_t(x)}{\Sigma_t^*}\right) = \frac{1}{\Delta x_i \Sigma_t^*} \frac{1}{N} \sum_n^N c_{n,i}^*, \tag{11}$$

where $c_{n,i}^*$ is the potential collision tally. To perform material-dependent collision tallies, tallies must be further normalized by the amount of material j in cell i: $\Delta x_{i,j}$. Because point-based material assignments are made in CoPS, the majority of the domain is not defined. An accurate but strenuous way to compute the material fractions seen in a cell would be to normalize material-dependent cell size using the fraction of tallied collisions for each material in cell i. We instead normalize for the ensemble-averaged, material-dependent flux cell size using the material abundance. We assume that CoPS does not sample a material preferentially over the other such that for a finite simulation, the proportion of materials sampled in each flux cell being near to the material abundance is highly probable. Flux tallies are then taken:

$$\phi_{i,j} = \frac{1}{\Delta x_{i,j} \Sigma_t^*} \frac{1}{N} \sum_n^N c_{n,i,j}^* = \frac{1}{\Delta x_i P_j \Sigma_t^*} \frac{1}{N} \sum_n^N c_{n,i,j}^*, \tag{12}$$

where P_j is the abundance of material j, $c_{n,i,j}^*$ is the potential collision tally for history n in cell i of material j, and $\Delta x_{i,j}$ is estimated as $\Delta x_i P_j$.

RESULTS AND ANALYSIS

We use CoPS to perform transport on a set of problem parameters for planar geometry from the benchmark suite provided in Ref. [1]. Table I shows the problem parameters, where $\Sigma_{t,j}$ is the total cross section, Λ_j is the average chord length, and c_j is the scattering ratio for each material $j \in \{0,1\}$. Only slab length $L = 10$ is considered.

TABLE I. Benchmark Set Parameters

Case Number	$\Sigma_{t,0}$	$\Sigma_{t,1}$	Λ_0	Λ_1
1	10/99	100/11	99/100	11/100
2	10/99	100/11	99/10	11/10
3	2/101	200/101	101/20	101/20
Case Letter	c_0	c_1		
a	0.0	1.0		
b	1.0	0.0		
c	0.9	0.9		

New benchmark results were produced in this paper using one history per realization, and they agree with published results within uncertainty. Table II provides the reflectance and transmittance results for each case for the benchmark approach (Bench) and CoPS method. Given in parentheses are the uncertainties (aka, standard error of the mean) on the last digit. Table II shows that overall, both mean reflectance

TABLE II. Reflectance and Transmittance Results for $L = 10.0$ Cases

Case		Reflectance		Transmittance	
		Bench	CoPS	Bench	CoPS
1	a	0.4360(4)	0.4281(4)	0.0148(1)	0.0163(1)
	b	0.08496(2)	0.0747(2)	0.00166(4)	0.00162(4)
	c	0.4777(4)	0.4514(4)	0.01631(1)	0.0167(1)
2	a	0.2372(4)	0.2338(4)	0.0980(2)	0.1001(3)
	b	0.2876(4)	0.2605(4)	0.1952(3)	0.1898(3)
	c	0.4326(4)	0.4072(4)	0.1870(3)	0.1904(3)
3	a	0.6904(4)	0.6824(4)	0.1639(3)	0.1723(3)
	b	0.0363(1)	0.0310(1)	0.0762(2)	0.0761(2)
	c	0.4451(4)	0.4212(4)	0.1042(3)	0.1067(3)

and transmittance results produced by CoPS closely align with benchmark results.

Both material-independent and material-dependent flux tallies were taken for each case. Here, we choose to show both the material-independent and material-dependent flux profiles produced by the benchmark method and CoPS for Cases 1b, 2c, and 3a in Figures 1 through 3, respectively. These figures show that the spatial flux distribution produced by CoPS agree with that produced using the benchmark method, demonstrating that CoPS can accurately perform both material-independent and material-dependent collision flux tallies. Other well-known approximate methods produce similar plots as seen in Ref. [2].

Figure 1 shows no pronounced differences in the flux profiles of Material 0 and Material 1. However, in both Figures 2 and 3, the distinction between the flux profiles in Material 0 and Material 1 is discernable and is not clearly captured from taking material-independent flux tallies alone. The relatively lower resolution of the flux distribution in Material 1 of Figure 2 is an artifact of fewer pseudo-collisions being sampled there due to the lower material abundance compared to Material 0.

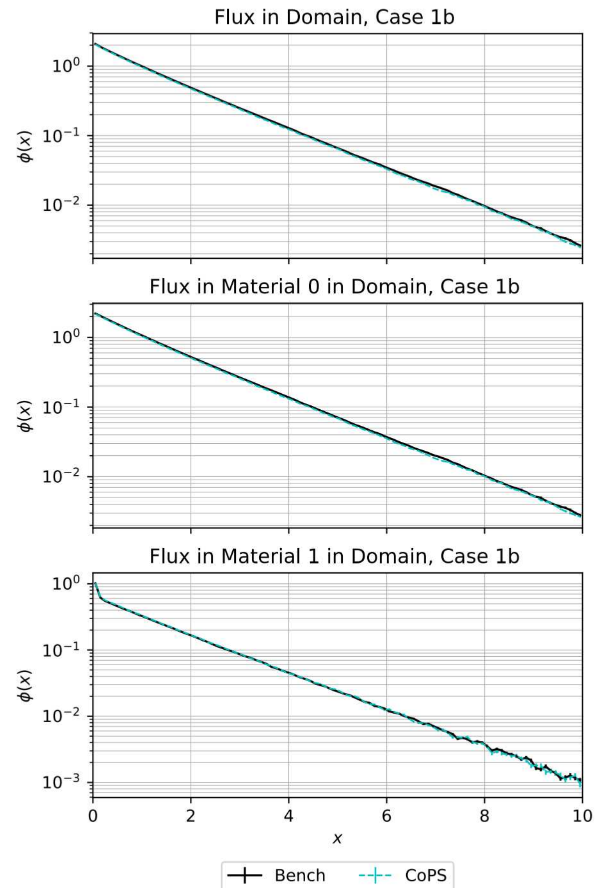

Fig. 1. Material-independent and material-dependent flux tally profile for Case 1b.

CONCLUSIONS AND FUTURE WORK

Woodcock tracking was used to perform radiation transport in one-dimensional, binary, Markovian-mixed media for planar geometries using a 2-point conditional probability function in Conditional Point Sampling (CoPS) on a set of problem parameters from the benchmark suite in Ref. [1]. The new method was demonstrated to produce mean leakage values and take both material-independent and material-dependent flux tallies. Mean transmittance, mean reflectance, and spatial flux distribution results were produced and shown to generally agree with benchmark results.

In the future, we hope to develop a more accurate, 3-point conditional probability function using the two nearest points. We plan to compare the accuracy of the mean and flux results produced by CoPS to other approximate methods for radiation transport in stochastic media and would like to implement an extension of the method to calculate the variance of the mean transport results due to the random material mixing. We

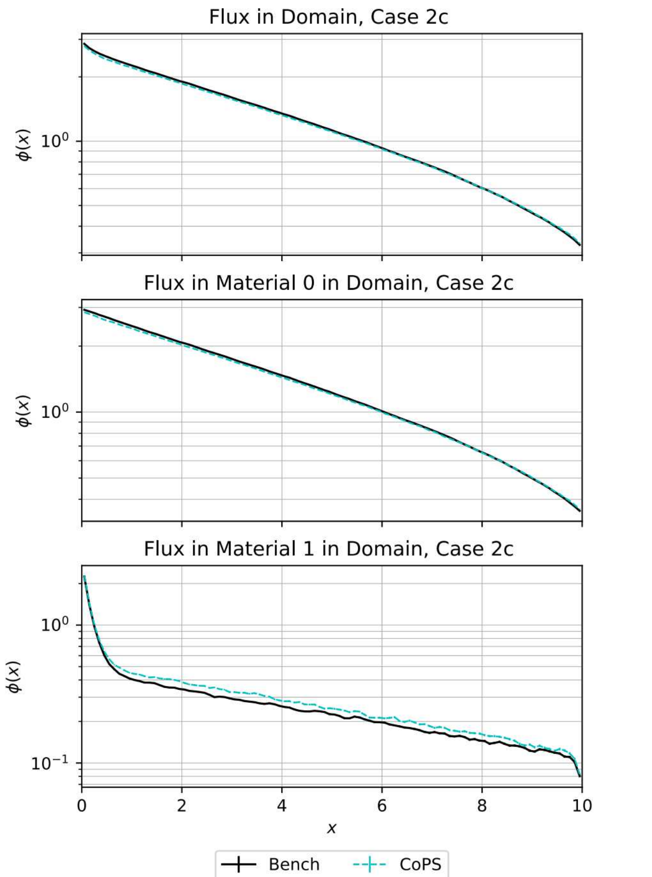

Fig. 2. Material-independent and material-dependent flux tally profile for Case 2c.

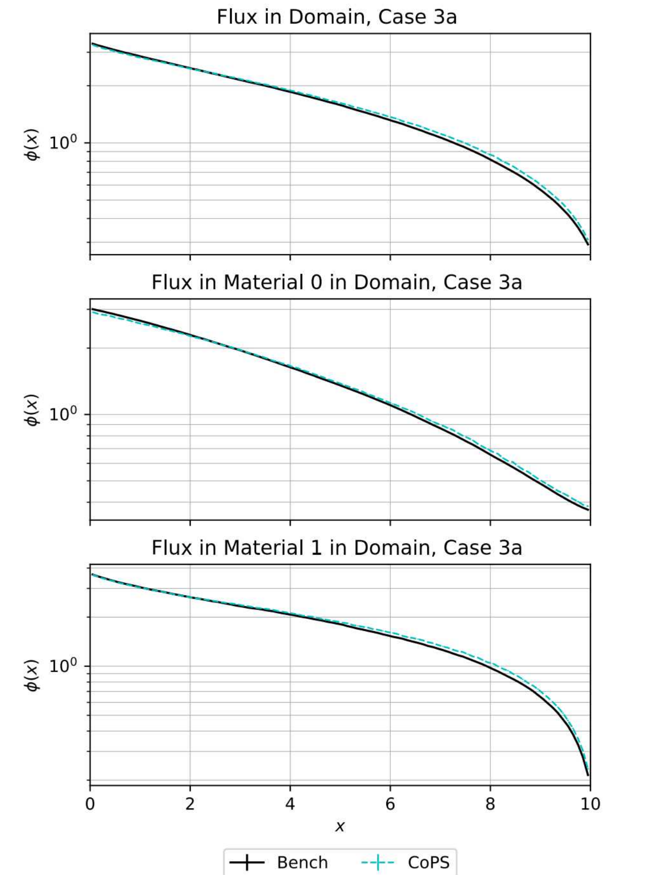

Fig. 3. Material-independent and material-dependent flux tally profile for Case 3a.

hope to port CoPS to multi-dimensional and multi-material geometries of arbitrary mixing types beyond Markovian-mixed media and further investigate the accuracy of those extensions.

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