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Recent Memory Versions of Conditional Point Sampling for Transport in 1D Stochastic Media

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INTRODUCTION

Conditional Point Sampling (CoPS) is a recently developed algorithm for computing radiation transport quantities in stochastic media. CoPS has some attractive qualities: a high degree of accuracy in 1D [1] and multi-D [2], ability to compute variance in outputs caused by material mixing [1], and exactness in 1D mixtures with Markovian mixing statistics [1]. However, it involves a list of points that grows during simulation causing potentially unbounded increases in runtime and memory requirements and is more complicated to understand and implement than some other notable approximate methods. In this summary, we investigate the accuracy of a simpler "recent memory" approach to CoPS that reduces runtime and memory and bears a resemblence to the well-known Chord Length Sampling [3, 4] (CLS).

The "benchmark" method of generating a large ensemble of material realizations and solving transport quantities on each of them was employed to establish the ensemble-averaged benchmark solutions. The atomic mix (AM) approximation [4] is evaluated by solving transport results on one realization that is a homogenization of the constituent materials. Chord Length Sampling (CLS) is the Monte Carlo version of the Levermore-Pomraning closure [3, 4, 5] and involves sampling, but not remembering, one material chord at a time. Memory-enhanced versions of CLS include "Algorithm B," also known as the Local Realization Preserving (LRP) [3, 4, 6] method, and "Algorithm C" (Alg. C) [3]. In 1D, LRP operates as CLS except that a material chord is remembered until the simulated particle exits the chord. Alg. C involves further memory by remembering the chord on each side in addition to the chord containing the particle.

In CoPS, rather than sampling material chords, material points are sampled on the fly. Delta tracking [7] is used such that the algorithm only needs to know what material it is interacting with at discrete pseudo-collision sites. The probability of sampling a particular material at a pseudo-collision site is based on material abundance and spatial correlation with points that have already been sampled. A conditional probability function incorporates these factors to determine the probabilities of sampling each possible material at a newly sampled point. To date, there are three primary versions of CoPS for 1D mixtures with Markovian mixing statistics [1] differentiated only by the conditional probability function used: CoPS2 (uses 2-point material correlations), CoPS3 (uses 3-point material correlations in a way easily extensible to multi-D [2]), and CoPS3PO (uses 3-point material correlations and is errorless for 1D, Markovian-mixed media; "PO" stands for "Pseudo-interface Optimum"). In each of these versions, all sampled material points are stored in computer memory and used in future conditional probability function evaluations.

In this summary, we investigate a simpler "recent memory" form of CoPS that stores only the sampled material assignments of the most recently visited locations by a history rather than that of every location. This simpler form trades accuracy for simplicity making the method more approachable–giving it a direct analogy to the celebrated Chord Length Sampling (CLS) method and derivatives–as well as faster-running and less memory intensive. In this study, we numerically investigate limited-memory versions of CoPS2 and CoPS3PO using the notation CoPSp-N to denote use of "p"-point material correlations based on the N most recently visited pseudo-collision sites, and compare its accuracy for several different user parameters to that of a collection of approximate methods on a common benchmark set [4, 5]. Results for all methods except the new limited memory CoPS were produced for Ref. [1] and reused here. It is the hope of the authors that this "recent memory" approach will improve theoretical and practical understanding of Conditional Point Sampling and play an impactful role in a broader "limited memory" scheme to come that maintains the attractive qualities of CoPS while reducing runtime and computer memory requirements.

THEORY

The following stochastic transport equation and boundary conditions describe transport in one-dimensional, binary, Markovian-mixed media on a slab geometry with an isotropic boundary source and otherwise vacuum boundary conditions:

$$\mu\frac{\partial\psi(x,\mu,\omega)}{\partial x}+\Sigma_t(x,\omega)\psi(x,\mu,\omega)=\frac{\Sigma_s(x,\omega)}{2}\int_{-1}^{1}d\mu'\psi(x,\mu',\omega), \quad (1a)$$

$$0\le x\le L,-1\le\mu\le 1; \quad (1b)$$

$$\psi(0,\mu)=2,\mu\ge 0,\psi(L,\mu)=0,\mu<0, \quad (1c)$$

where x and μ are the particle spatial and angular variables, respectively, ω is the material realization, and L is the length of the domain.

A common way to generate a Markovian-mixed realization is by successively sampling chord lengths beginning at a boundary [4, 5]. Another method is based on the property that the average number of pseudo-interfaces, I, per slab length r is Poisson-distributed [8]. The average number of pseudo-interfaces is

$$I=\frac{r}{\Lambda_c}, \quad (2)$$

where in binary media, the correlation length Λ_c is computed using Λ_α and Λ_β, the average chord lengths of materials α and

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β, respectively [8]:

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

The number of pseudo-interfaces in a particular realization is computed using the frequency of k pseudo-interfaces

$$f(k, I) = \frac{I^k}{k!} e^{-I}, \tag{4}$$

and each pseudo-interface is distributed in a realization using a spatially uniform distribution. The material type of each cell defined by these pseudo-interfaces is sampled using material abundances. For binary media composed of materials α and β, the abundance or probability of sampling materials α and β, respectively, are

$$P_\alpha = \frac{\Lambda_\alpha}{\Lambda_\alpha + \Lambda_\beta}, \tag{5a}$$

$$P_\beta = 1 - P_\alpha. \tag{5b}$$

CONDITIONAL POINT SAMPLING

In Conditional Point Sampling (CoPS), the use of delta tracking [7] enables on-the-fly material point assignments. The algorithm begins by initializing the particle position and direction, x and μ. A streaming even is selected by taking the minimum of the distance to boundary and distance to potential collision, $d_c^* = -\frac{1}{\Sigma_t^*} \ln(\xi)$, where Σ_t^* is the largest total cross section (i.e. the majorant cross section) in the domain, and ξ is a randomly generated number uniformly sampled between 0 and 1. If the particle streams to a potential collision, the potential collision is accepted by sampling against the probability of a true collision, expressed as the ratio between the true and majorant cross sections: $P_{col} = \frac{\Sigma_t}{\Sigma_t^*}$.

The material type at a potential collision site is sampled using the material abundance (Eq. 5a) if no other points have been defined. However, if other point-based material assignments have already been made, a derived conditional probability function specific to the domain's governing spatial statistics is used to sample the material type at the new point conditionally on neighboring points. For one-dimensional, binary, Markovian-mixed media, conditional probability functions dependent on only the nearest point or only the nearest point on each side of a new point were derived in Ref. [1]. "CoPS2" uses a 2-point conditional probability function to compute the probability of sampling material α at a new point (in which κ denotes that the material type hasn't been sampled yet) conditionally on knowing the material type of the point at distance r_1 away:

$$\pi(\alpha, \alpha|\alpha, \kappa) = 1 - P_\beta\left(1 - e^{-\frac{r_1}{\Lambda_c}}\right), \tag{6a}$$

$$\pi(\beta, \alpha|\beta, \kappa) = P_\alpha\left(1 - e^{-\frac{r_1}{\Lambda_c}}\right). \tag{6b}$$

"CoPS3PO," in which the "PO" stands for pseudo-interface optimum, uses a 3-point conditional probability function based on the nearest point on each side of a new point that is errorless for 1D binary materials with Markovian mixing statistics. The probability of sampling material α at the new point based on points of material type m_1 and m_2 distances r_1 and r_2 away on the left and right, respectively are

$$\pi(\alpha, \alpha, \alpha|\alpha, \kappa, \alpha) = 1 - \frac{P_\beta\left(1 - e^{-\frac{r_1}{\Lambda_c}}\right)\left(1 - e^{-\frac{r_2}{\Lambda_c}}\right)}{1 - \frac{P_\beta}{P_\beta - 1} e^{-\frac{r_1 + r_2}{\Lambda_c}}}, \tag{7a}$$

$$\pi(\beta, \alpha, \beta|\beta, \kappa, \beta) = \frac{P_\alpha\left(1 - e^{-\frac{r_1}{\Lambda_c}}\right)\left(1 - e^{-\frac{r_2}{\Lambda_c}}\right)}{1 - \frac{P_\alpha}{P_\alpha - 1} e^{-\frac{r_1 + r_2}{\Lambda_c}}}, \tag{7b}$$

$$\pi(\alpha, \alpha, \beta|\alpha, \kappa, \beta) = \frac{\left(1 - e^{-\frac{r_2}{\Lambda_c}}\right)\left[1 - P_\beta\left(1 - e^{-\frac{r_1}{\Lambda_c}}\right)\right]}{1 - e^{-\frac{r_1 + r_2}{\Lambda_c}}}, \tag{7c}$$

In "CoPS3" an alternative derivation and notation are used that are straightforward to extend to multi-D [2]. CoPS3 is not as accurate as CoPS3PO in 1D; the two versions of CoPS are compared in more detail in Ref. [1]. The probability of sampling material α at the new point based on the nearest, non-excluded points is denoted $\pi(\alpha|\boldsymbol{m})$ where $\boldsymbol{m} = \{m_1, m_2, ..\}$ is a vector containing the material types of the points and $\boldsymbol{r} = \{r_1, r_2, ...\}$ is a vector of distances to the points:

$$\pi(\alpha|\{\alpha, \alpha\}) = 1 - P_\beta\left(1 - e^{-\frac{r_1}{\Lambda_c}}\right)\left(1 - e^{-\frac{r_2}{\Lambda_c}}\right), \tag{8a}$$

$$\pi(\alpha|\{\beta, \beta\}) = P_\alpha\left(1 - e^{-\frac{r_1}{\Lambda_c}}\right)\left(1 - e^{-\frac{r_2}{\Lambda_c}}\right), \tag{8b}$$

$$\pi(\alpha|\{\alpha, \beta\}) = \frac{\left(1 - e^{-\frac{r_2}{\Lambda_c}}\right)\left[1 - P_\beta\left(1 - e^{-\frac{r_1}{\Lambda_c}}\right)\right]}{1 - e^{-\frac{r_1 + r_2}{\Lambda_c}}}. \tag{8c}$$

RESULTS AND ANALYSIS

Here, we present results produced using the 2-point (CoPS2) and errorless 3-point (CoPS3PO) implementations of CoPS that remember a maximum of $N = 0, 1, 2, 3, 10, 50$ and 100 most recent points using 1E6 particle histories for a set of problem parameters provided in Ref. [5]. CoPSp-1 draws analogy to CLS in that each new point is sampled based only on knowledge of the most recently visited point similar to how CLS samples each new chord based only on knowledge of which material type the particle is in. CoPSp-N for $N > 1$ is analogous to memory-enhanced versions of CLS, i.e., LRP and Algorithm C, in that additional memory of previously sampled geometry features are remembered. In the limit as $N \to \infty$, the original versions of CoPS are recovered; for brevity CoPSp-∞ is simply denoted CoPSp.

The problem parameters of Tables 10-18 in Ref. [5] for planar geometry are listed in Table I, 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. To compare the accuracy of each method, the relative error is calculated using

$$E_R = \frac{x_{approx} - x}{x}, \tag{9}$$

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

where x is the benchmark leakage value and x_{approx} is the leakage value computed by the various solvers. The root mean squared (RMS), mean absolute, and maximum absolute relative error of leakage results are computed for each solver over the benchmark:

$$\text{RMS } E_R = \sqrt{\frac{1}{N}\sum_i E_{R_i}^2}, \tag{10}$$

$$\text{Mean}|E_R| = \frac{1}{N}\sum_i |E_{R_i}|, \tag{11}$$

$$\text{Max}|E_R| = \max |E_{R_i}|. \tag{12}$$

Table II provides reproduced mean leakage results using the benchmark, CoPS2, CoPS3, and CoPS3PO methods from Ref. [1]. CoPS2, CoPS3, and CoPS3PO results from this reference were produced by remembering all points defined throughout a particle history, which is effectively CoPSp-∞. This table also provides CoPS2-N mean leakage results up to $N = 3$. In Table III are the root mean squared (RMS), mean, and maximum relative error of established approximate methods produced in Ref. [1] and of CoPS2-N up to $N = 3$. In parentheses are the statistical uncertainties (i.e. standard error of the mean) on the last digit. Figure 1 shows the behavior in RMS E_R for CoPS2 and CoPS3PO as a function of points remembered compared to other approximate methods for reflectance and transmittance.

In Table III and Figure 1, CoPS2 and CoPS3PO are similar in accuracy to the atomic mix (AM) approximation when remembering zero points and to Chord Lenght Sampling (CLS) when remembering one point for both reflectance and transmittance. Remembering more recent points improves the accuracy of CoPS monotonically with the upper limit of accuracy being that achieved by CoPS when remembering all points. For reflectance, CoPS3PO achieves comparable accuracy to LRP and CoPS2 at $N = 50$, and at $N = 100$, it approaches the accuracy of Alg. C. When remembering a maximum of 100 points, CoPS2-N approaches its accuracy limit (CoPS2-∞). For transmittance, CoPS2 and CoPS3PO achieve an accuracy close to that of LRP for $N = 5$. CoPS2-50 is almost as accurate as Alg. C while CoPS3PO-50 surpasses it. At $N = 100$, CoPS3PO surpasses the accuracy of CoPS2-∞.

CONCLUSIONS

The accuracy of recent memory versions of Conditional Point Sampling (CoPS) remembering N most recent material points were investigated using 2-point and errorless 3-point

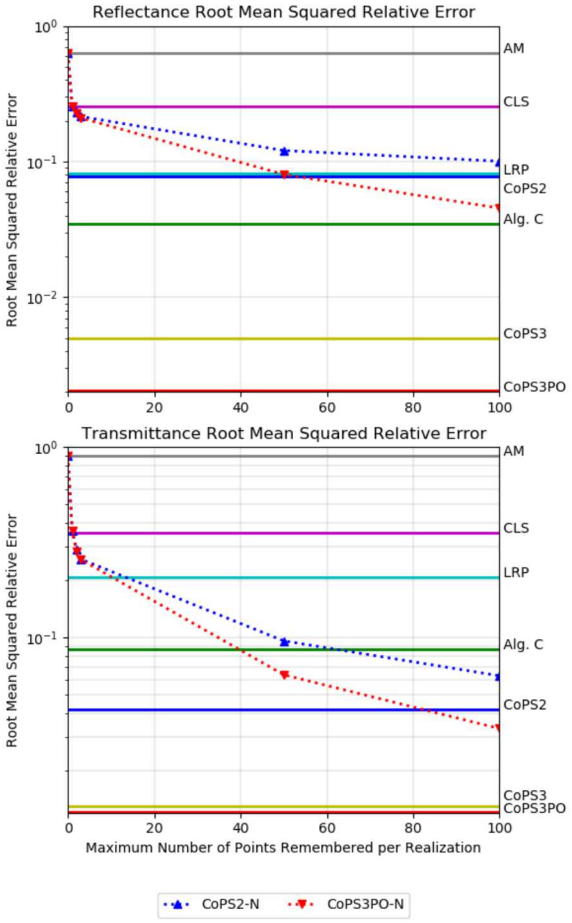

Fig. 1. Reflectance (top) and transmittance (bottom) root mean squared error of results across benchmark set

conditional probability functions on a common benchmark suite. Accuracy was compared to other approximate methods. Notably, CoPS2 and CoPS3PO were roughly as accurate as the atomic mix approximation for $N = 0$ and Chord Length Sampling for $N = 1$. Increasing the number of points remembered monotonically increased the accuracy; at 100 points remembered, the accuracy was meaningfully improved over few points remembered but had not yet reached the accuracy achieved when remembering all points.

In the future, we plan to investigate other memory reduction techniques in CoPS designed to retain a high degree of accuracy while improving runtime and memory efficiency as well as hybrids of new techniques with the recent memory technique presented here. After evaluating the accuracy of various limited-memory techniques in 1D, we plan to compare their runtimes and extend to multi-D.

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TABLE II. Computed CoPSp-N Reflectance and Transmittance Results

$\langle L \rangle$	Case	Bench [1]	CoPS2-0	CoPS2-1	CoPS2-2	CoPS2-3	CoPS2 [1]	CoPS3 [1]	CoPS3PO [1]
$\langle R \rangle$	1a	0.4360(5)	0.4951(5)	0.3778(5)	0.3894(5)	0.3951(5)	0.4282(5)	0.4372(5)	0.4368(5)
	1b	0.0850(3)	0.0196(1)	0.0584(2)	0.0590(2)	0.0594(2)	0.0747(3)	0.0846(2)	0.0849(3)
	1c	0.4778(5)	0.4778(5)	0.3694(5)	0.3888(5)	0.3955(5)	0.4514(5)	0.4785(4)	0.4775(5)
	2a	0.2373(5)	0.4957(5)	0.1804(4)	0.1913(4)	0.1984(4)	0.2339(4)	0.2375(4)	0.2375(4)
	2b	0.2876(5)	0.0198(1)	0.2182(4)	0.2187(4)	0.2189(4)	0.2605(4)	0.2862(5)	0.2865(5)
	2c	0.4326(5)	0.4778(5)	0.2889(5)	0.3157(5)	0.3295(5)	0.4073(5)	0.4332(5)	0.4332(5)
	3a	0.6904(5)	0.7861(4)	0.6068(5)	0.6226(5)	0.6307(5)	0.6825(5)	0.6903(5)	0.6903(5)
	3b	0.0364(2)	0.00197(4)	0.0242(2)	0.0242(2)	0.0245(2)	0.0310(2)	0.0360(2)	0.0363(2)
	3c	0.4452(5)	0.4778(5)	0.3268(5)	0.3508(5)	0.3632(5)	0.4212(5)	0.4436(5)	0.4447(5)
$\langle T \rangle$	1a	0.0149(1)	0.00468(7)	0.0265(2)	0.0239(2)	0.0229(1)	0.0163(1)	0.0148(1)	0.0149(1)
	1b	0.00167(5)	0.000008(3)	0.00149(4)	0.00157(4)	0.0015(4)	0.00163(4)	0.00162(5)	0.00163(4)
	1c	0.0163(1)	0.00389(6)	0.0239(2)	0.0225(1)	0.0221(1)	0.0168(1)	0.0160(1)	0.0159(1)
	2a	0.0980(3)	0.00468(7)	0.1284(3)	0.1227(3)	0.1185(3)	0.1002(3)	0.0982(3)	0.0983(3)
	2b	0.1953(4)	0.000012(3)	0.1794(4)	0.1794(4)	0.1802(4)	0.1898(4)	0.1957(3)	0.1958(4)
	2c	0.1870(4)	0.00389(6)	0.1953(4)	0.1973(4)	0.1988(4)	0.1905(4)	0.1871(4)	0.1870(4)
	3a	0.1639(4)	0.0668(2)	0.2400(4)	0.2254(4)	0.2172(4)	0.1723(4)	0.1644(4)	0.1643(4)
	3b	0.0762(3)	0.000010(3)	0.0760(3)	0.0756(3)	0.0756(3)	0.0762(3)	0.0763(3)	0.0763(3)
	3c	0.1042(3)	0.00387(6)	0.1195(3)	0.1176(3)	0.1173(3)	0.1067(3)	0.1040(3)	0.1039(3)

TABLE III. Reflectance and Transmittance Ensemble Error Metrics of Reproduced Results [1] and Computed CoPSp-N Results

$\langle L \rangle$	Error	AM	CLS	LRP	Alg. C	CoPS2	CoPS3	CoPS3PO	CoPS2-0	CoPS2-1	CoPS2-2	CoPS2-3
$\langle R \rangle$	RMS E_R	0.631	0.257	0.080	0.035	0.078	0.005	0.002	0.632	0.256	0.229	0.215
	Mean $\lvert E_R \rvert$	0.465	0.246	0.069	0.021	0.064	0.003	0.001	0.465	0.245	0.216	0.200
	Max $\lvert E_R \rvert$	1.088	0.341	0.148	0.087	0.146	0.011	0.004	1.089	0.335	0.334	0.325
$\langle T \rangle$	RMS E_R	0.894	0.355	0.207	0.087	0.042	0.013	0.012	0.893	0.362	0.288	0.257
	Mean $\lvert E_R \rvert$	0.881	0.260	0.139	0.045	0.033	0.008	0.008	0.881	0.267	0.216	0.197
	Max $\lvert E_R \rvert$	1.000	0.765	0.489	0.239	0.099	0.030	0.026	1.000	0.779	0.610	0.538

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