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BENCHMARK COMPARISONS OF MONTE CARLO ALGORITHMS FOR ONE-DIMENSIONAL N-ARY STOCHASTIC MEDIA

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ABSTRACT

We extend the Monte Carlo Chord Length Sampling (CLS) and Local Realization Preserving (LRP) algorithms to the N-ary stochastic medium case using two recently developed uniform and volume fraction models that follow a Markov-chain process for N-ary problems in one-dimensional, Markovian-mixed media. We use the Lawrence Livermore National Laboratory Mercury Monte Carlo particle transport code to compute CLS and LRP reflection and transmission leakage values and material scalar flux distributions for one-dimensional, Markovian-mixed quaternary stochastic media based on the two N-ary stochastic medium models. We conduct accuracy comparisons against benchmark results produced with the Sandia National Laboratories PlaybookMC stochastic media transport research code. We show that CLS and LRP produce exact results for purely absorbing N-ary stochastic medium problems and find that LRP is generally more accurate than CLS for problems with scattering.

KEYWORDS: Monte Carlo, stochastic medium, Levermore-Pomraning, Chord Length Sampling, Local Realization Preserving

1. INTRODUCTION

A primary focus in stochastic media transport has been one-dimensional, binary, Markovian-mixed problems [1], and approximate methods such as the Atomic Mix (AM) approximation [1], Chord Length Sampling (CLS), Local Realization Preserving (LRP) [2,3], Algorithm C (Alg. C) [2], and Conditional Point Sampling (CoPS) [4] have been developed to handle this type of problem. The accuracy of these approximate methods has been assessed using a set of problem parameters and benchmarks established in Ref. [5]. The AM approximation is one of the most well-known approximate methods and homogenizes the material properties within a domain for an ensemble of realizations. However, the method generally lacks accuracy for problems with a correlation length that deviates significantly from zero. When using exponentially distributed chord lengths, CLS is the

Monte Carlo equivalent of the Levermore-Pomraning (LP) closure [2,3,5] and is exact for purely-absorbing problems. The method samples material chords on-the-fly and forgets the sampled chord length after each particle streaming event. LRP and Alg. C are memory-enhanced versions of CLS and are generally more accurate than CLS for problems involving scattering. CoPS uses delta tracking [6] to sample point-based material types on-the-fly conditionally on neighboring material points. The accuracy of CoPS is dependent on the fidelity of the conditional probability function used, which is derived based on a "pseudo-interface" approach of generating realizations [7] and is specific to the material-mixing type of the domain.

Research efforts have, of late, shifted significantly to expanding stochastic media transport comparisons beyond one dimension for AM, CLS, LRP [8] and CoPS [9] using benchmarks published by Larmier et al. [10]. In addition, Poisson-Box Sampling (PBS) [11] is a new method developed for multi-dimensional geometries that samples, in real-time, the material type of "Cartesian boxes" that are generated using Poisson-distributed hyperplanes in Cartesian-coordinate directions. In Ref. [11], two variants of PBS algorithms, analogous to CLS and LRP in one dimension (1D), were investigated: one that committed the material type and geometric definition of the current Cartesian box to computer memory (PBS-1) and one that committed the material type and geometric definition of the current and most recent Cartesian box to computer memory (PBS-2).

Limited previous research has been performed in expanding capabilities to more than two materials. Pautz and Franke [12] produced a set of benchmark results for N-ary Markovian-mixed problems in 1D based on early theoretical work in material mixing [13,14]. Olson et al. [15] has recently investigated the theory of N-ary, Markovian-mixing and has identified two models for N-ary mixtures that contain self-consistent material-mixing statistics satisfying Markov-chain properties and that reduce to long-established properties of binary, Markovian-mixed media [1]: one uses a uniform sampling approach to sample the material type of successive chords while the other uses volume fraction sampling. In this work, we use corresponding uniform and volume fraction sampling schemes based on the models established in Ref. [15] to extend CLS and LRP to N-ary stochastic medium problems for one-dimensional, Markovian-mixed media. We compute reflection and transmission leakage values and material scalar flux distributions using the Lawrence Livermore National Laboratory Mercury Monte Carlo particle transport code [16]. We compare the accuracy of those results to benchmark results produced using the Sandia National Laboratories stochastic media transport code called PlaybookMC, which has capabilities for N-ary geometries and was previously used in Ref. [4] to reproduce established 1D, binary, Markovian-mixed benchmark suite results from Refs. [2,3,5] using the benchmark method, AM approximation, CLS, LRP, and Alg. C to conduct accuracy comparisons against results produced using the CoPS algorithm.

The remainder of this paper is organized as follows. We first describe the stochastic particle transport equation for one-dimensional, N-ary, stochastic media and the models used for N-ary media in Section 2. We then describe the extension of the Monte Carlo algorithms investigated in this paper to N-ary media in Section 3 and briefly describe a set of benchmark problem parameters used for this study in Section 4. We then present numerical results and accuracy comparisons in Section 5 and conclude with a discussion and suggestions for future work in Section 6.

2. THEORY

Transport in one-dimensional, N-ary, Markovian-mixed media in planar geometry, with isotropic scattering, and with an isotropic boundary source and otherwise vacuum boundary conditions can be described with the following stochastic transport equation:

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

$$0\leq x\leq L, -1\leq\mu\leq 1,$$

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

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

The notation is standard with the exception of the variable ω representing the stochastic dependence of the material properties.

To generate N-ary material realizations in one-dimensional geometries, material chord lengths can be sampled successively beginning at a boundary using the self-consistent models established in Ref. [15]. In this work, we generate quaternary realizations using both the uniform and volume fraction sampling schemes discussed in Ref. [15]. Both models reduce to the same standard material-mixing statistics for binary, Markovian-media established in Ref. [1] and preserve input mean chord lengths and volume fractions for the sampled material realizations.

The uniform sampling scheme samples successive chord lengths based on a material type determined using a uniform distribution that excludes the current material the particle is in:

$$P(j|i)=\frac{1}{N-1}, \tag{2a}$$

where N is the number of material types in the problem, i is the current material type, and $i\neq j$. The uniform sampling model assumes that the material volume fractions, p_i, are computed as:

$$p_i=\frac{\Lambda_i}{\sum\limits_{j=0}^{N-1}\Lambda_j}, \tag{2b}$$

where Λ_i and Λ_j are the mean chord lengths of material i and j, respectively. The uniform sampling scheme has no constraints on the mean chord length values. This sampling method does not appear to be easily extensible to multi-dimensional problems for the generation of material realizations [15].

The volume fraction sampling scheme samples successive chord lengths based on a material type determined using a weighted probability that excludes the current material probability:

$$P(j|i)=\frac{p_j}{1-p_i}, \tag{3a}$$

where i is the current material type and $i\neq j$. The volume fractions are computed using

$$p_i=1-\frac{\Lambda_c}{\Lambda_i} \iff \Lambda_c<\Lambda_i, \tag{3b}$$

where the expression for the correlation length, Λ_c, is determined using Eq. (3b) along with the requirement that the volume fractions sum to unity:

$$\Lambda_c = \frac{N-1}{\sum_{i=0}^{N-1} \frac{1}{\Lambda_i}}. \tag{3c}$$

Because the material volume fractions must be positive, Eq. (3b) implies the constraint that $\Lambda_c < \Lambda_i$ for this sampling method. This sampling method produces 1D realizations that are statistically equivalent to 1D realizations producible using the hyperplane-based method employed in 3D in Refs. [10] and [11] and established for N-ary mixing in Ref. [15].

3. MONTE CARLO ALGORITHMS

Ref. [3] describes in detail the Monte Carlo Chord Length Sampling (CLS) and Local Realization Preserving (LRP) algorithms for 1D, binary stochastic media. Ref. [2] introduces the distance to material interface event, $d_i = -\Lambda_i \ln(\xi)/|\mu|$, where ξ is a uniform random number and μ is the particle direction cosine with respect to the x-axis. Here, we describe the extension of each algorithm to N-ary stochastic media using the two sampling schemes described in Section 2.

The particle track for each history in CLS is as follows:

1. Sample the distance to material interface, d_i, with the material type sampled in proportion to volume fraction.
   (a) If using the uniform sampling scheme, compute volume fractions using Eq. (2b).
   (b) If using the volume fraction sampling scheme, compute volume fractions using Eq. (3b).
2. Compute the distance to boundary, d_b, and sample the distance to collision, d_c.
3. Determine the particle event by computing the minimum of d_i, d_b, and d_c and stream particle.
   (a) If the boundary is crossed, terminate particle.
   (b) If the particle event is a collision event, sample the collision type. Terminate the particle if absorbed. Otherwise, return to step 1.
   (c) If the material interface is crossed, sample a new d_i. Return to step 2.
      i. If using the uniform sampling scheme, sample material type using Eq. (2a).
      ii. If using the volume fraction sampling scheme, sample material type using Eq. (3a).

The particle track for each history in LRP is as follows:

1. Sample the distance to material interface in the forward and backward direction, d_i^+ and d_i^-, respectively, with the material type sampled in proportion to volume fraction.
   (a) If using the uniform sampling scheme, compute volume fractions using Eq. (2b).
   (b) If using the volume fraction sampling scheme, compute volume fractions using Eq. (3b).

2. Compute the distance to boundary, d_b, and sample the distance to collision, d_c.
3. Determine the particle event by computing the minimum of d_i^+, d_b, and d_c and stream particle.
   (a) If the boundary is crossed, terminate particle.
   (b) If the particle event is a collision event, sample the collision type. Terminate the particle if absorbed. Otherwise, adjust the distance to interface in the forward and backward direction to account for the change in angle after scattering, and switch d_i^+ and d_i^- in the event of backscattering. Return to step 2.
   (c) If the material interface is crossed, sample a new d_i^+ and set d_i^- to zero. Return to step 2.
      i. If using the uniform sampling scheme, sample material type using Eq. (2a).
      ii. If using the volume fraction sampling scheme, sample material type using Eq. (3a).

4. BENCHMARK SUITE DESCRIPTION

We consider a planar geometry benchmark suite corresponding to Eqs. (1a)–(1c) involving an isotropic angular flux incident on a quaternary stochastic medium. The problem parameters investigated in this paper are adapted from the benchmark suite described in Ref. [5] for planar geometry. Table 1 shows the cross section parameters used for each of the twelve problems investigated (three case numbers times four case letters), where $\Sigma_{t,i}$ [cm^{-1}] and $c_i = \Sigma_{s,i}/\Sigma_{t,i}$ are the total cross section and scattering ratio, respectively, for material $i \in \{0, 1, 2, 3\}$. A slab thickness of $L = 10$ cm is used for all cases.

Table 1: Benchmark Suite Cross Section Parameters

Case Number	$\Sigma_{t,0}$	$\Sigma_{t,1}$	$\Sigma_{t,2}$	$\Sigma_{t,3}$	Case Letter	c_0	c_1	c_2	c_3
1	10/99	100/11	10/99	100/11	a	1.0	0.0	1.0	0.0
2	2/101	200/10	2/101	200/101	b	0.0	1.0	0.0	1.0
3	10/99	100/11	2/101	200/101	c	0.9	0.9	0.9	0.9
					d	0.0	0.0	0.0	0.0

Tables 2 and 3 show the volume fractions, p_i, and mean chord lengths, Λ_i [cm], for material $i \in \{0, 1, 2, 3\}$ for each case for the uniform and volume fraction sampling schemes, respectively. Table 3, which gives values for the volume fraction sampling scheme, also shows the correlation length Λ_c [cm] for each case. Because the volume fraction sampling scheme has a constraint that limits the mean chord lengths allowed, the two sampling schemes in this paper are evaluated using consistent volume fractions.

For the parameters used for the uniform sampling scheme, shown in Table 2, we use mean chord lengths inspired by the mean chord lengths in the benchmark suite in Ref. [5]. In Table 2, we also show the derived material volume fractions computed from the mean chord lengths using Eq. (2b).

For the parameters used for the volume fraction sampling scheme, we use the same set of material volume fractions as for the uniform sampling scheme. However, using the same set of mean chord lengths as for the uniform sampling scheme would result in a violation of the constraint imposed by Eq. (3c) that $\Lambda_c < \Lambda_i$. Therefore, we compute the derived mean chord lengths from the material volume fractions using Eq. (3b) by choosing an arbitrary correlation length for each case number. Note that although the same volume fractions are used for both material sampling schemes, each model uses different sets of mean chord lengths except for the "2" cases for which using a correlation length of $\Lambda_c = 303/80$ cm with the volume fractions listed for Case 2 for the volume fraction sampling scheme yields the same mean chord lengths used for the uniform sampling.

Table 2: Benchmark Suite Material Parameters for Uniform Sampling

Case Number	Derived Material Volume Fraction				Mean Chord Length			
	p_0	p_1	p_2	p_3	Λ_0	Λ_1	Λ_2	Λ_3
1	9/110	1/110	9/11	1/11	99/100	11/100	99/10	11/10
2	1/4	1/4	1/4	1/4	101/20	101/20	101/20	101/20
3	99/1120	11/1120	101/224	101/224	99/100	11/100	101/20	101/20

Table 3: Benchmark Suite Material Parameters for Volume Fraction Sampling

Case Number	Material Volume Fraction				Derived Mean Chord Length				Correlation Length
	p_0	p_1	p_2	p_3	Λ_0	Λ_1	Λ_2	Λ_3	Λ_c
1	9/110	1/110	9/11	1/11	110/101	110/109	11/2	11/10	1
2	1/4	1/4	1/4	1/4	101/20	101/20	101/20	101/20	303/80
3	99/1120	11/1120	101/224	101/224	1680/1021	1680/1109	112/41	112/41	3/2

5. RESULTS AND ANALYSIS

In this section, we present reflection and transmission leakage values and material-dependent scalar flux distributions for the one-dimensional, quaternary, Markovian-mixed media benchmark suite defined in Section 4. The benchmark results used to conduct accuracy comparisons were produced using the Sandia National Laboratories PlaybookMC research code [4]. The Monte Carlo CLS and LRP leakage and scalar flux results presented in this paper were produced using the Lawrence Livermore National Laboratory Mercury Monte Carlo particle transport code [16]. (As additional verification, the Mercury results were compared with CLS and LRP values produced using PlaybookMC and found to agree to within one standard deviation.) The material-dependent scalar flux distributions were tallied in 100 bins of size $\Delta x = 0.1$ cm. All results were produced using 10^7 particle histories. We compute the relative error for each benchmark case using

$$E_R = \frac{x - x_{approx}}{x}, \tag{4}$$

where x is the benchmark result and x_{approx} is the result produced using the approximate method. We compute the root mean squared relative error, mean absolute relative error, and maximum absolute relative error across the entire benchmark suite for the reflection and transmission results of each approximate method:

$$\text{RMS}E_R = \sqrt{\frac{1}{N_c}\sum_i E_{R_i}^2}, \tag{5a}$$

$$\text{Mean}|E_R| = \frac{1}{N_c}\sum_i |E_{R_i}|, \tag{5b}$$

$$\text{Max}|E_R| = \max|E_{R_i}|, \tag{5c}$$

where N_c is the total number of cases not including purely absorbing results and E_{R_i} is the relative error of case i. Note that purely absorbing results were excluded entirely from the computation of these error metrics since the CLS and LRP algorithms are exact (to within statistical uncertainty) for purely absorbing problems.

Table 4 shows the mean reflection and transmission values produced using the benchmark (Bench) approach, CLS, and LRP for both the uniform and volume fraction sampling schemes. The standard error of the mean (1σ) on the last digit is shown in parentheses. Table 4 shows that for purely-absorbing problems ("d" cases), CLS and LRP produce exact results within statistical uncertainty. Results produced using the uniform sampling scheme agree with results produced using the volume fraction sampling scheme for all "2" cases for which the same set of material probabilities and mean chord lengths are used. Table 5 shows the computed error metrics of each method for the benchmark suite. The relative errors of the purely absorbing leakage results ("d" cases) were not included in these computations. Table 5 shows that LRP is generally more accurate than CLS in computing reflection and transmission leakage values for this set of benchmark problems.

Material-dependent scalar flux distributions were produced for each problem using both sampling schemes. Figures 1 and 2 show the material-dependent scalar flux distributions for Case 1d using the uniform sampling scheme and Case 3c using the volume fraction sampling scheme, respectively, where the standard deviations in the flux distributions are less than 1.5% for all spatial bins. Figure 1 shows that for a purely-absorbing problem, Case 1d, CLS and LRP produce exact material-dependent scalar flux distributions. Figure 2 illustrates that for a problem with scattering, LRP generally produces more accurate scalar flux distributions than CLS due to the algorithm's local memory of the sampled chord length. Although generally more accurate, the scalar flux distributions produced by LRP are not always more accurate than CLS at all points in space. Full characterization of the relative accuracy of the flux distributions produced by CLS and LRP for N-ary stochastic medium problems requires further investigation in future work.

6. CONCLUSIONS

In this paper, we extended the Monte Carlo Chord Length Sampling (CLS) and Local Realization Preserving (LRP) algorithms to N-ary stochastic materials for one-dimensional, Markovian-mixed media using uniform and volume fraction sampling schemes based on the models established in Ref [15]. We demonstrated that CLS and LRP can be successfully extended to N-ary stochastic media by computing mean reflection and transmission leakage results and scalar flux distributions

Table 4: Mean Leakage Results

Sampling Scheme	Case	Reflection Bench	Reflection CLS	Reflection LRP	Transmission Bench	Transmission CLS	Transmission LRP
Uniform	1a	0.2942(1)	0.2318(1)	0.2748(1)	0.2231(1)	0.2073(1)	0.2207(1)
	1b	0.2230(1)	0.1748(1)	0.1925(1)	0.1084(1)	0.1336(1)	0.1244(1)
	1c	0.4260(1)	0.3023(2)	0.3625(2)	0.2148(1)	0.2197(1)	0.2294(1)
	1d	0.0000(0)	0.0000(0)	0.0000(0)	0.08914(9)	0.08891(9)	0.08918(8)
	2a	0.04482(7)	0.03153(6)	0.03886(6)	0.1318(1)	0.1304(1)	0.1314(1)
	2b	0.6522(2)	0.5748(2)	0.6041(2)	0.2019(1)	0.2737(1)	0.2469(1)
	2c	0.4225(2)	0.3140(2)	0.3630(2)	0.1561(1)	0.1690(1)	0.1735(1)
	2d	0.0000(0)	0.0000(0)	0.0000(0)	0.1099(1)	0.10998(9)	0.11011(9)
	3a	0.05457(7)	0.03563(6)	0.04467(7)	0.1031(1)	0.1017(1)	0.10249(9)
	3b	0.6203(2)	0.5437(2)	0.5669(2)	0.1663(1)	0.2228(2)	0.2054(1)
	3c	0.4351(2)	0.3241(2)	0.3646(2)	0.1325(1)	0.1468(1)	0.1516(1)
	3d	0.0000(0)	0.0000(0)	0.0000(0)	0.0837(1)	0.0836(1)	0.08360(8)
Volume Fraction	1a	0.2880(1)	0.2192(1)	0.2478(1)	0.1974(1)	0.1811(1)	0.1893(1)
	1b	0.2362(1)	0.1797(1)	0.2202(1)	0.09913(9)	0.12879(9)	0.10724(9)
	1c	0.4324(2)	0.2896(1)	0.3786(1)	0.1882(1)	0.1961(1)	0.2048(1)
	1d	0.0000(0)	0.0000(0)	0.0000(0)	0.07820(8)	0.07827(7)	0.07857(8)
	2a	0.04451(7)	0.03156(6)	0.03874(6)	0.1318(1)	0.1304(1)	0.1315(1)
	2b	0.6520(2)	0.5746(2)	0.6041(2)	0.2022(1)	0.2739(1)	0.2470(1)
	2c	0.4225(2)	0.3140(1)	0.3625(2)	0.1559(1)	0.1691(1)	0.1736(1)
	2d	0.0000(0)	0.0000(0)	0.0000(0)	0.1101(1)	0.1100(1)	0.1103(1)
	3a	0.04405(6)	0.02866(5)	0.03654(5)	0.03434(6)	0.03361(6)	0.03409(6)
	3b	0.6745(1)	0.5915(2)	0.6288(2)	0.1169(1)	0.1794(1)	0.1496(1)
	3c	0.4633(2)	0.3421(1)	0.4019(2)	0.06312(8)	0.07836(8)	0.07677(8)
	3d	0.0000(0)	0.0000(0)	0.0000(0)	0.02680(5)	0.02679(5)	0.02679(5)

for a benchmark suite adapted from that in Ref. [5], and we conducted accuracy comparisons using benchmark values produced using Sandia National Laboratories' research code PlaybookMC. We showed that CLS and LRP produce exact results for purely absorbing cases and that LRP is generally more accurate than CLS using both the uniform and volume fraction sampling schemes. In future work, we hope to extend these N-ary stochastic medium capabilities in CLS and LRP to multi-dimensional problems.

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Table 5: Mean Leakage Relative Error

Sampling Scheme	Error Metric	Reflection CLS	Reflection LRP	Transmission CLS	Transmission LRP
Uniform	RMS E_R	0.246	0.131	0.189	0.135
	Mean$\|E_R\|$	0.235	0.125	0.137	0.105
	Max$\|E_R\|$	0.347	0.181	0.356	0.235
Volume Fraction	RMS E_R	0.257	0.122	0.253	0.150
	Mean$\|E_R\|$	0.245	0.116	0.186	0.117
	Max$\|E_R\|$	0.349	0.170	0.535	0.280

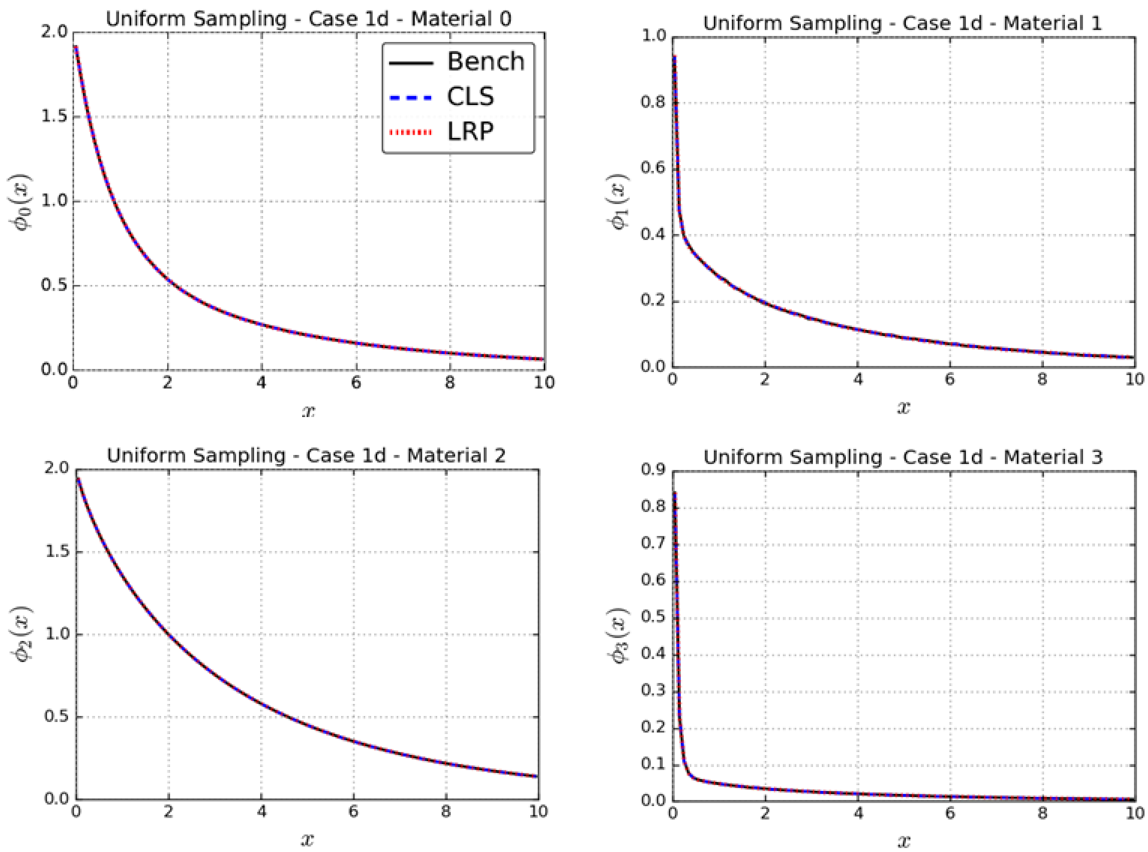

Figure 1: Case 1d material-dependent scalar flux distributions using the uniform sampling scheme

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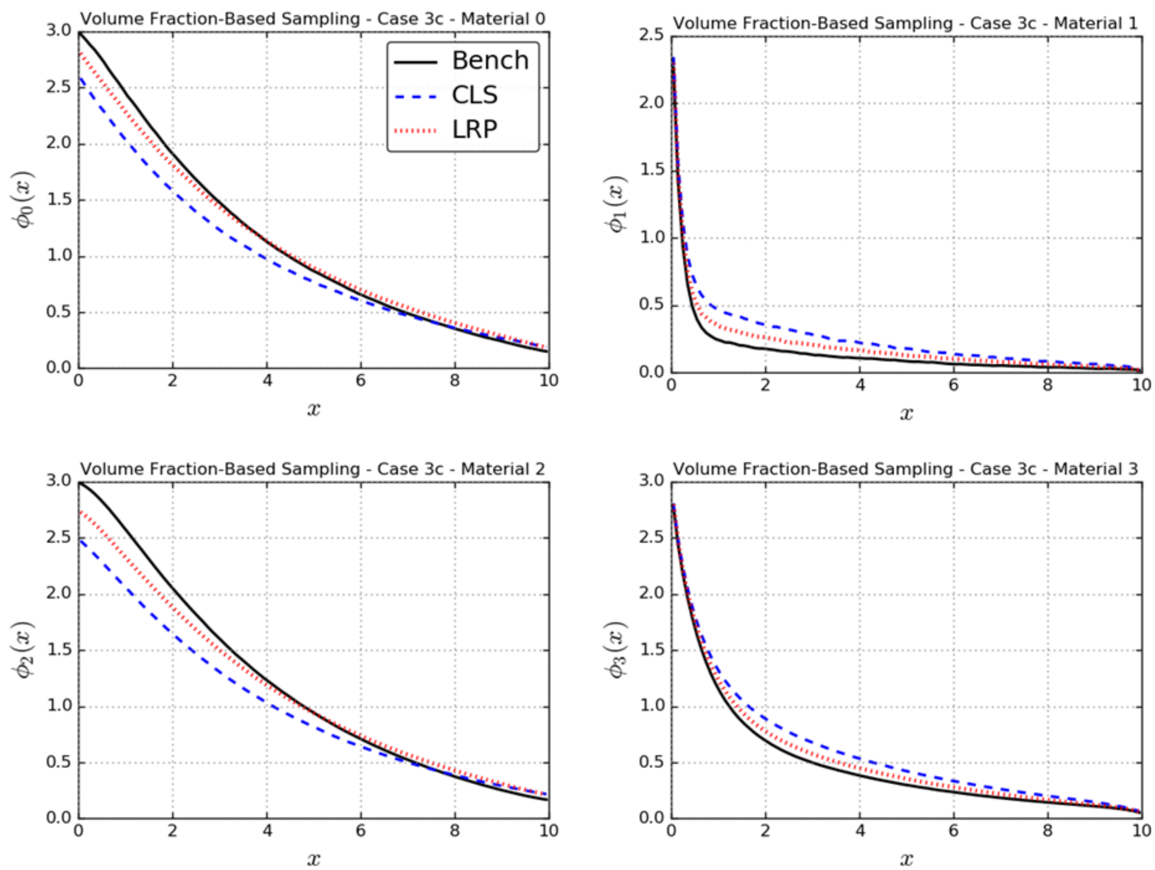

Figure 2: Case 3c material-dependent scalar flux distributions using the volume fraction sampling scheme

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