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Benchmark Comparisons of Monte Carlo Algorithms for One-Dimensional N-ary Stochastic Media

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Emily H. Vu, Patrick S. Brantley, Aaron J. Olson (SNL), and Brian C. Kiedrowski (UM)

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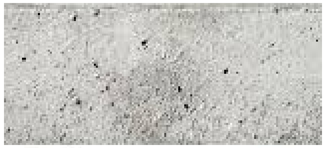
Lawrence Livermore National Laboratory

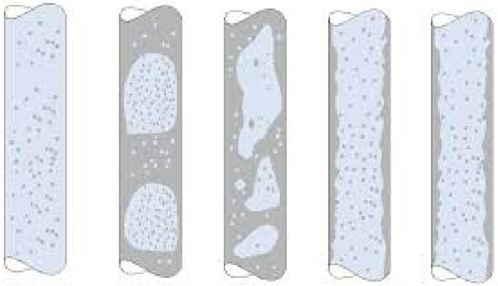
Outline

- **Introduction and Background**
- N-ary Material-Mixing Models
- Monte Carlo Algorithms
- Problem Description and Results and Analysis
- Conclusions and Future Work

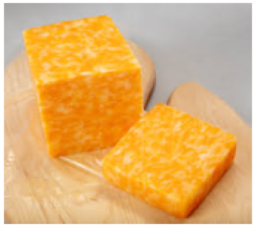
Introduction and Background
Stochastic Media

- Spatially heterogenous mixing
  - BWR Coolant
  - Concrete
  - Rayleigh-Taylor instabilities
  - Pebble Bed Reactors (PBR)





- Cheese
  - Smoked Gouda (atomically mixed)
  - Colby Jack (binary)
  - Pepper Jack (N-ary)



Introduction and Background
Methods for One-Dimensional, Binary, Markovian-Mixed Media

- Benchmark (bench)
  - (M. L. Adams, E. W. Larsen, and G. C. Pomraning, 1989)
  - Brute force method that performs transport on ensemble of realizations
  - Exact but slow to converge
- Atomic Mix (AM) approximation
  - (P.S. Brantley, 2011)
  - Mixing at atomic level
  - Exact in the limit of small mean chord lengths (autocorrelation = 0)
- Algorithm A – Chord Length Sampling (CLS)
  - (G. B. Zimmerman and M. L. Adams, 1991)
  - Monte Carlo equivalent of Levermore-Pomraning Closure
  - Exact for purely absorbing media
  - No memory of chord length after each particle segment
- Algorithm B – Local Realization Preserving (LRP)
  - (G. B. Zimmerman and M. L. Adams, 1991) and (P. S. Brantley and G. B. Zimmerman, 2017)
  - Remembers current chord length until particle leaves current material
- Algorithm C
  - (G. B. Zimmerman and M. L. Adams, 1991)
  - Remembers current chord length and chord lengths on each side
- Conditional Point Sampling (CoPS)
  - (E.H. Vu and A.J. Olson, 2021)
  - Two components: algorithm (errorless) and conditional probability function
  - Uses Woodcock tracking to make discrete point-wise material designations in real-time

Introduction and Background

Extension to d-Dimensional, Binary, Markovian-Mixed Media

- Benchmark (bench)
- Atomic Mix (AM) approximation
- Algorithm A – Chord Length Sampling (CLS)
- Algorithm B – Local Realization Preserving (LRP)
- **Algorithm C (Alg. C)**
- Conditional Point Sampling (CoPS)
- Poisson-Box Sampling (PBS)
  - (C. Larmier, A. Zoia, F. Malvagi, E. Dumonteil, and A. Mazzolo., 2018)
  - Defines “Cartesian boxes” using Poisson-distributed hyperplanes in Cartesian-coordinate directions
  - Samples material type of Cartesian boxes on-the-fly
  - Memory versions of PBS (PBS-1 and PBS-2) analogous to LRP and Alg. C

Introduction and Background

Extension to One-Dimensional, N-ary, Markovian-Mixed Media

- S. D. Pautz and B. C. Franke. *"The Levermore-Pomraning and Atomic Mix closures for n-ary stochastic materials."* M&C 2017, on USB (2017).
  - Produced transport benchmark results
  - Work based on theoretical work of:
    - R. Sanchez (1989).
    - O. Zuchuat, R. Sanchez, I. Zmijarevic, and F. Malvagi (1994)
    - G. C. Pomraning (1991)

- A. J. Olson, S. D. Pautz, D. S. Bolintineanu, and E. H. Vu. *"Theory and generation methods for N -ary stochastic mixtures with Markovian mixing statistics."* M&C 2021 (2021).
  - Provides general framework for N-ary mixtures that form a Markov-chain process. Two types of Markovian mixtures are the
    - Uniform Sampling Model
    - Volume Fraction Sampling Model
  - Both models recover input mean chord lengths, volume fractions, and other measurable descriptors in sampled material realizations.
  - Both models reduce to the established binary, Markovian-mixed model (Pomraning, 1991).

In this work, we investigate two material sampling schemes based on the models in (Olson et al., 2021) using Monte Carlo algorithms CLS and LRP.

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Material-Mixing Models:
Stochastic Transport Equation for Planar Geometry

- Stochastic Transport Equation

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

- Boundary Conditions

$$0 \le x \le L; -1 \le \mu \le 1$$
$$\psi(0,\mu) = 2, \mu \ge 0; \psi(L,\mu) = 0, \mu < 0$$

- Nomenclature
  - L – domain length
  - x, μ, ω – spatial, angular, and stochastic dependence
  - $\Sigma_t(x,\omega)$ – total cross section
  - $\psi(x,\mu,\omega)$ – angular flux

Material-Mixing Models:
Binary Markovian-Mixed Media Mixing Statistics

- Chord Length Distribution

$$\lambda_\alpha = -\Lambda_\alpha \log \xi$$
$$\lambda_\beta = -\Lambda_\beta \log \xi$$

- Correlation Length

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

- Material Volume Fraction

$$P_\alpha = \frac{\Lambda_\alpha}{\Lambda_\alpha + \Lambda_\beta}$$
$$P_\beta = 1 - P_\alpha$$

- Material Probability at Interface

$$\pi(\alpha|\beta) = 1$$
$$\pi(\beta|\alpha) = 1$$

Material-Mixing Models:
N-ary Markovian-Mixed Media Mixing Statistics – Uniform Sampling

- Chord Length Distribution

$$\lambda_i = -\Lambda_i \log \xi$$

- Material Volume Fraction

$$P_i = \frac{\Lambda_i}{\sum_j^N \Lambda_j}$$

- Material Probability at Interface

$$\pi(j|i) = \frac{1}{N-1}$$

Material-Mixing Models:

N-ary Markovian-Mixed Media Mixing Statistics – Volume Fraction Sampling

- Chord Length Distribution

$$\lambda_i = -\Lambda_i \log \xi$$

- Correlation Length

$$\Lambda_c = \frac{N-1}{\sum_i^N \frac{1}{\Lambda_i}}$$

- Material Volume Fraction

$$P_i = 1 - \frac{\Lambda_c}{\Lambda_i}, \qquad \Lambda_c < \Lambda_i$$

- Material Probability at Interface

$$\pi(j|i) = \frac{P_j}{1 - P_i}$$

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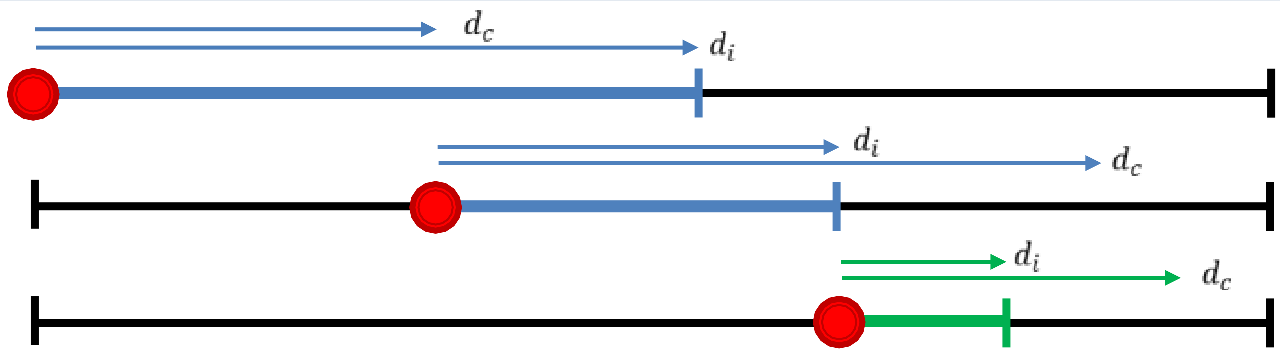
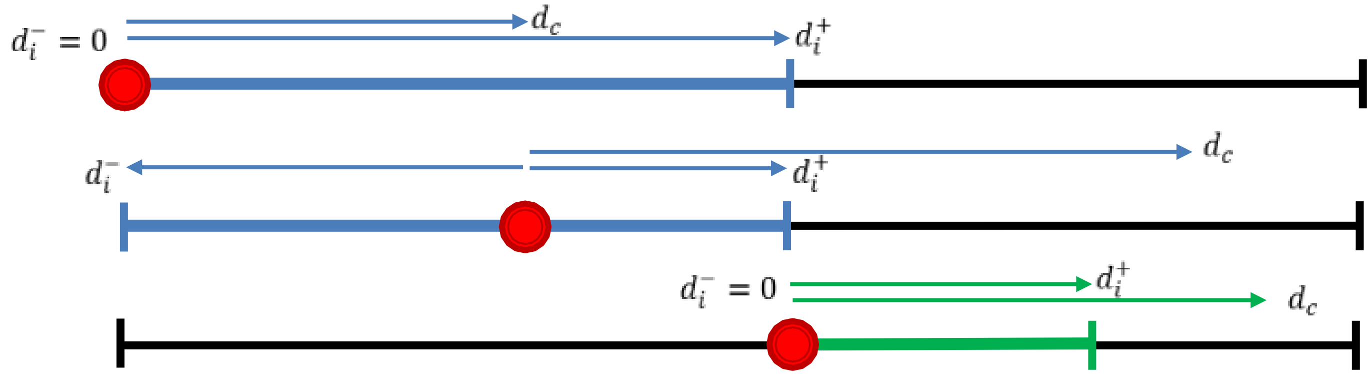
Monte Carlo Algorithms:
Chord Length Sampling (CLS)



1) Sample distance to material interface, d_i, with the material type sampled in proportion to volume fraction.
   1) Uniform Sampling: $P_i = \frac{\Lambda_i}{\sum_j^N \Lambda_j}$
   2) Volume Fraction Sampling: $P_i = 1 - \frac{\Lambda_c}{\Lambda_i}$
2) Compute distance to boundary, d_b, and sample distance to collision, d_c.
3) Determine particle event by computing the minimum of d_i, d_c, and d_b and stream particle.
   1) If boundary is crossed, terminate particle.
   2) If minimum distance is to collision event, sample collision type. Terminate particle if absorbed. Return to step 2.
   3) If material interface is crossed, sample a new d_i. Return to step 2.
      1) Uniform Sampling: $\pi(j|i) = \frac{1}{N-1}$
      2) Volume Fraction Sampling: $\pi(j|i) = \frac{P_j}{1-P_i}$

Monte Carlo Algorithms:
Local Realization Preserving (LRP)



1) Sample 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.
   1) Uniform Sampling: $P_i = \frac{\Lambda_i}{\sum_j^N \Lambda_j}$
   2) Volume Fraction Sampling: $P_i = 1 - \frac{\Lambda_c}{\Lambda_i}$
2) Compute distance to boundary, d_b, and sample distance to collision, d_c.
3) Determine particle event by computing the minimum of d_i, d_c, and d_b and stream particle.
   1) If boundary is crossed, terminate particle.
   2) If minimum distance is to collision event, sample collision type. Terminate particle if absorbed. Otherwise, adjust d_i^+ and d_i^-. In case of backscatter, switch d_i^+ and d_i^-. Return to step 2.
   3) If material interface is crossed, sample new d_i^+ and set d_i^- to zero. Return to step 2.
      1) Uniform Sampling: $\pi(j|i) = \frac{1}{N-1}$
      2) Volume Fraction Sampling: $\pi(j|i) = \frac{P_j}{1-P_i}$

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Problem Description:
Benchmark Suite Problem Parameters

- Benchmark Set 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

- Results
  - Benchmark results produced using PlaybookMC
  - CLS and LRP results produced using Mercury
  - Results produced using 1E7 particles

Problem Description:
Benchmark Suite Problem Parameters for Each Sampling Scheme

- Benchmark Set 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

- Benchmark Set 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

Results and Analysis:
Computed Error Metrics

- Relative Error

$$E_R = \frac{x - x_{approx}}{x}$$

- Root Mean Squared Relative Error

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

- Mean Absolute Relative Error

$$Mean\ |E_R| = \frac{1}{N}\sum_i |E_{R_i}|$$

- Maximum Absolute Relative Error

$$Max|E_R| = \max |E_{R_i}|$$

Results and Analysis:

Generated Mean Leakage Benchmarks – Uniform Sampling 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)

- CLS and LRP produce statistically errorless results for purely absorbing problems (“d” cases).

Results and Analysis:

Generated Mean Leakage Benchmarks – Volume Fraction Sampling Results

Sampling Scheme	Case	Reflection			Transmission		
		Bench	CLS	LRP	Bench	CLS	LRP
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)

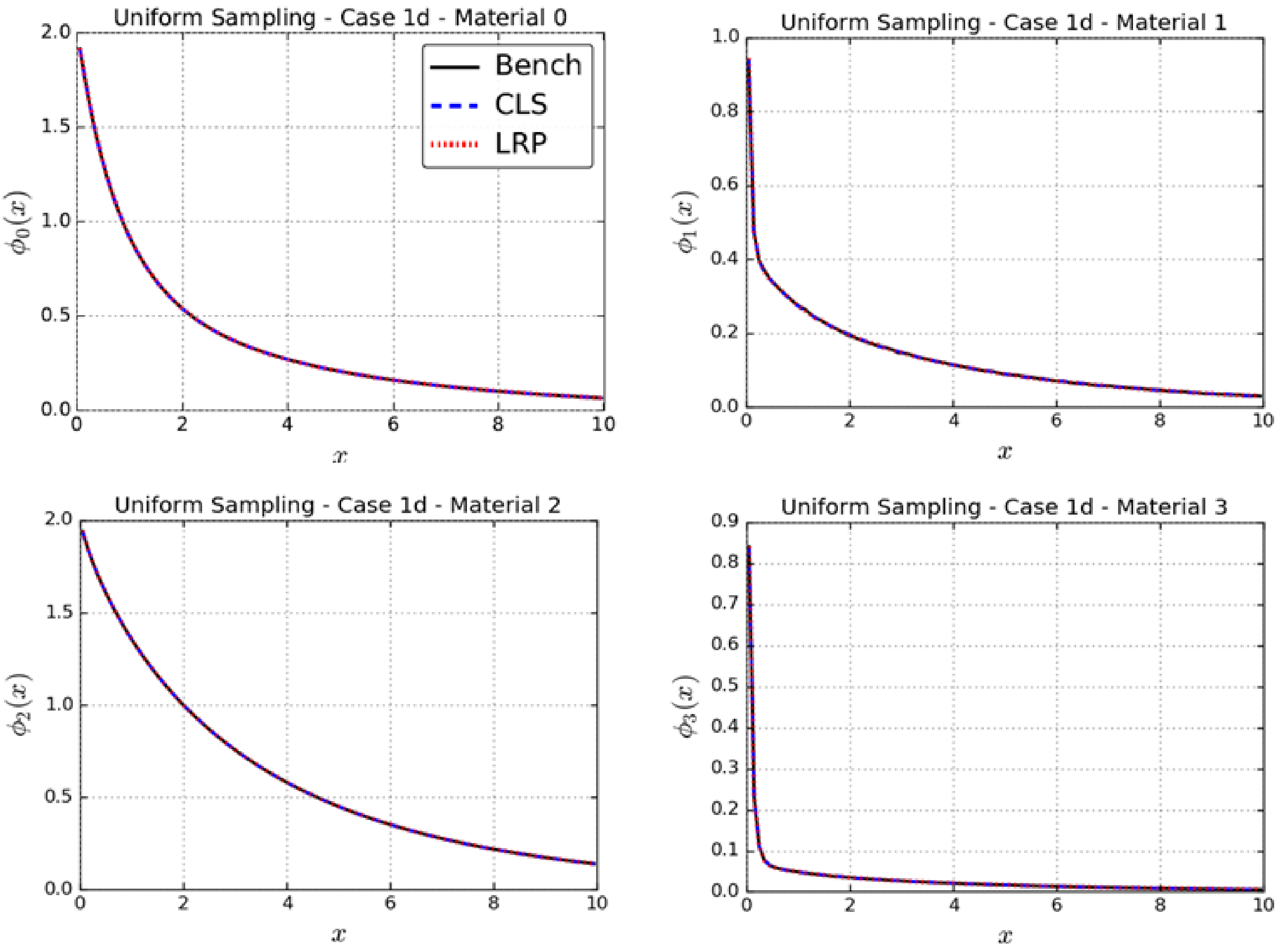
- CLS and LRP produce statistically errorless results for purely absorbing problems ("d" cases).

Results and Analysis:
Mean Leakage Accuracy Comparison – Computed Error Metrics

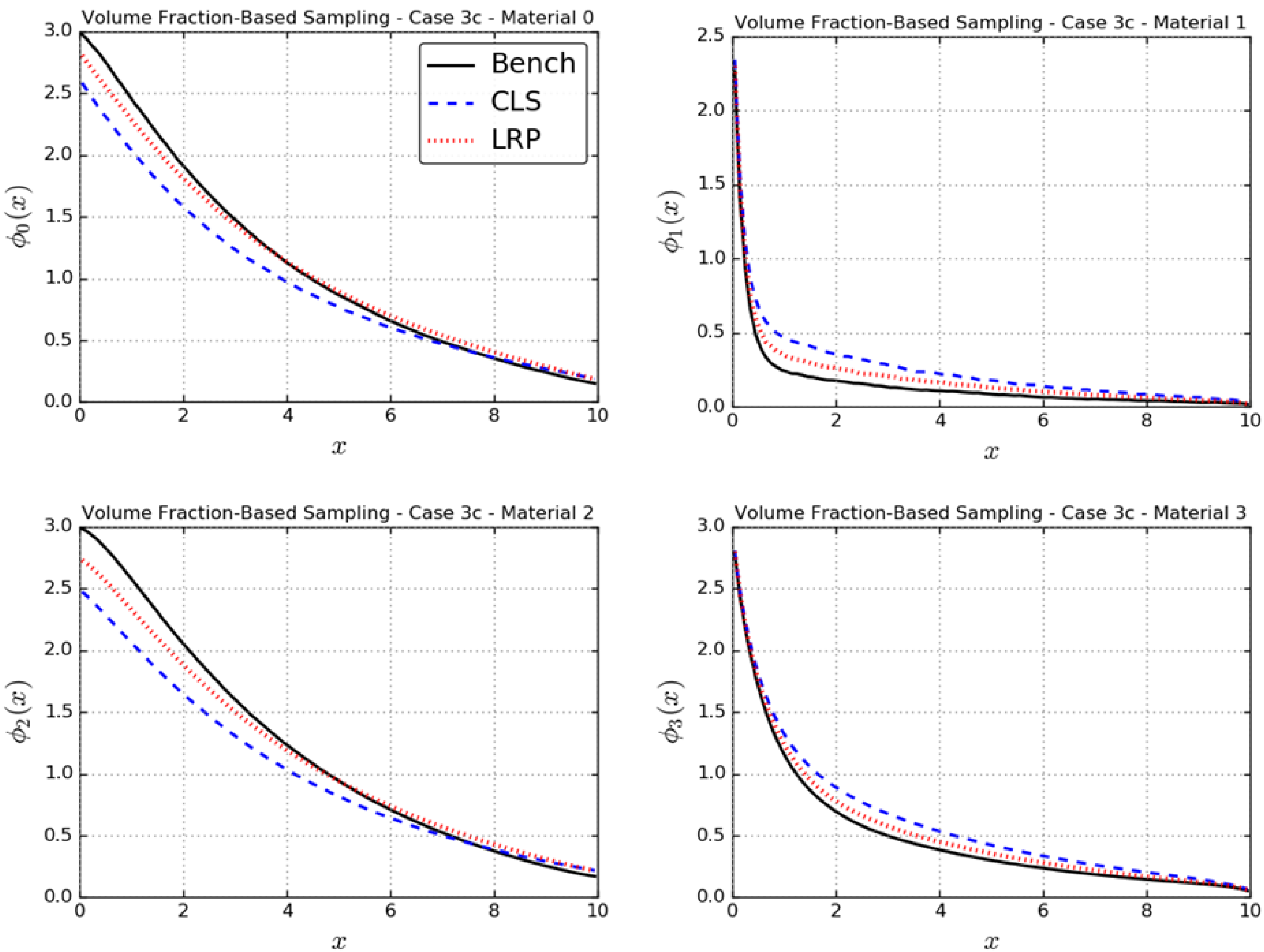
Sampling Scheme	Error Metric	Reflection CLS	Reflection LRP	Transmission CLS	Transmission LRP
Uniform	RMS E_R	0.246	0.131	0.189	0.135
	Mean$\lvert E_R \rvert$	0.235	0.125	0.137	0.105
	Max$\lvert E_R \rvert$	0.347	0.181	0.356	0.235
Volume Fraction	RMS E_R	0.257	0.122	0.253	0.150
	Mean$\lvert E_R \rvert$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

- The relative error of purely absorbing leakage results ("d" cases) were not included in computation.
- LRP is more accurate than CLS for this set of benchmark problems.

Results and Analysis:
Scalar Flux Distributions: Case 1d – Uniform Sampling



Results and Analysis:
Scalar Flux Distributions: Case 3c – Volume Fraction Sampling



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Conclusions and Future Work

- Conclusions
  - Demonstrated Chord Length Sampling (CLS) and Local Realization Preserving (LRP) to extend to N-ary stochastic medium for one-dimensional planar geometry
  - Assessed accuracy of CLS and LRP algorithms by comparing mean leakage results and material scalar flux distributions to benchmark results
  - Uniform and volume fraction-based sampling schemes are self-consistent for each set of problem parameters
  - CLS and LRP produce exact results for purely absorbing problems
  - LRP is generally more accurate than CLS for the problems examined

- Future Work
  - Extend N-ary CLS and LRP to multi-dimensional problems

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