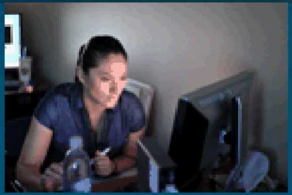
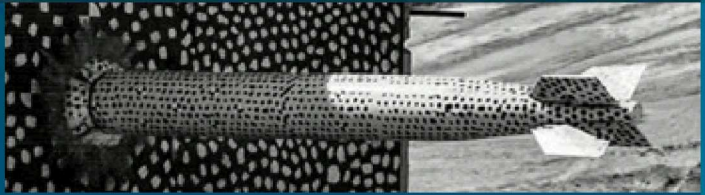
SAND2019-6299C

Conditional Point Sampling: A Novel Monte Carlo Method for Radiation Transport in Stochastic Media





PRESENTED BY

Emily H. Vu and Aaron J. Olson

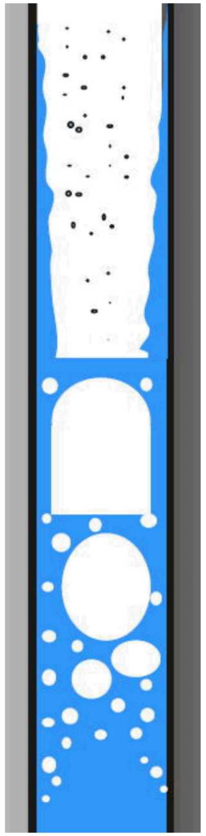
Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Outline

- **Introduction and Problem Statement**
- Example Use of Conditional Point Sampling Approach
- Conditional Point Sampling Analysis
- Conclusion and Future Work

Stochastic Media

- Spatially heterogenous mixing
  - Random material type
  - Rayleigh-Taylor instabilities
  - BWR Coolant
  - Porous materials



Problem Statement

- Stochastic Transport Equation

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

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

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

- x, μ, ω – spatial, angular, and stochastic dependence
- $\Sigma_t(x,\omega)$ – total cross section
- $\Sigma_s(x,\mu,\omega)$ – angular cross section
- L – domain length
- Isotropic boundary source on “left” boundary, otherwise vacuum BCs

Markovian-Mixed Media Statistics

- Correlation length based on chord lengths of each material $(\Lambda_\alpha, \Lambda_\beta)$:

$$\Lambda_c = \frac{\Lambda_\alpha \Lambda_\beta}{\Lambda_\alpha + \Lambda_\beta} \tag{2}$$

- Average number of pseudo-interfaces per distance r:

$$I = \frac{r}{\Lambda_\mathrm{c}} \tag{3}$$

- Pseudo-interfaces are Poisson-distributed, so their frequency is:

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

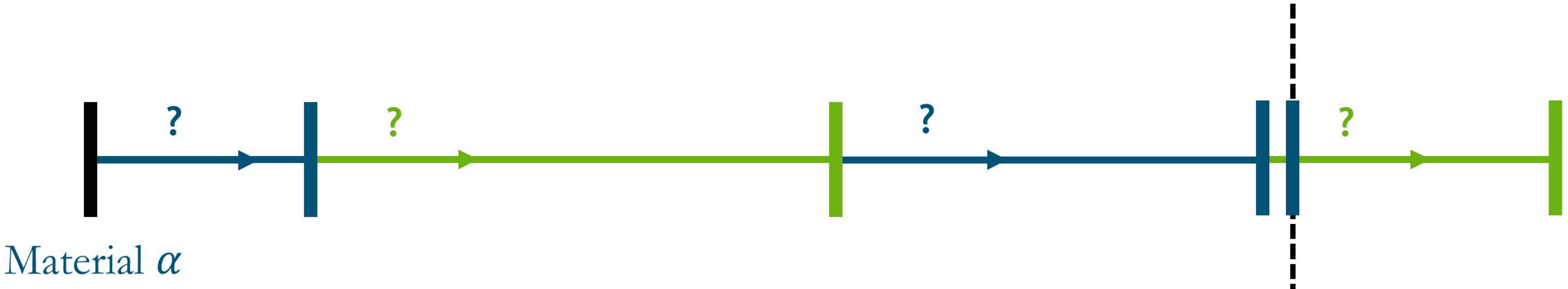
- Probability of material at a random point in a realization:

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

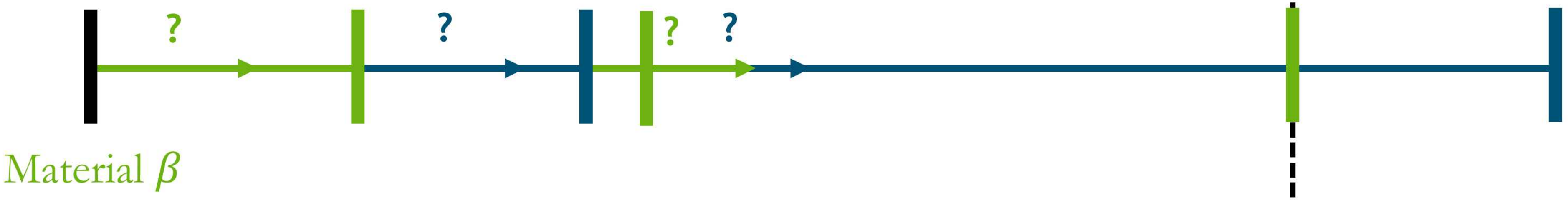
Constructing Binary Markovian-Mixed Media Common Method

Material α (dark blue)
Material β (green)

$$P_\alpha = \frac{\Lambda_\alpha}{\Lambda_\alpha + \Lambda_\beta}; P_\beta = 1 - P_\alpha = \frac{\Lambda_\beta}{\Lambda_\alpha + \Lambda_\beta}; \lambda_{\alpha,i} = \Lambda_\alpha \log\left(\frac{1}{\xi}\right)$$



Two materials Λ_α and Λ_β.
Sample against to determine material type.
Sample chord length $\lambda_{\alpha,i}$.



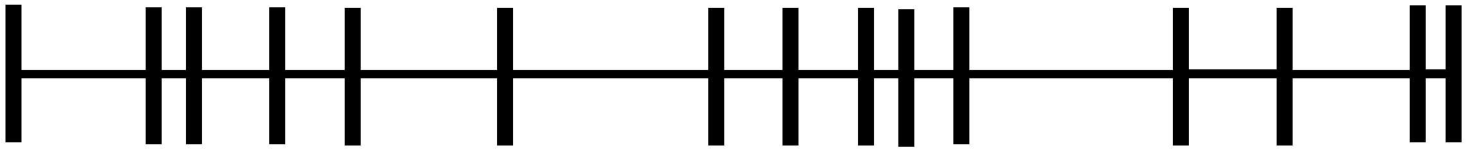
Constructing Binary Markovian-Mixed Media: Less Common Method

Material α

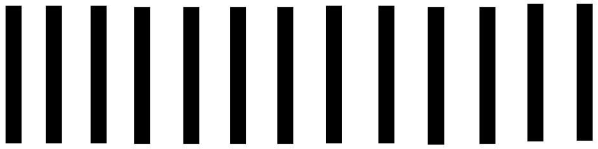
Material β

$$P_\alpha = \frac{\Lambda_\alpha}{\Lambda_\alpha + \Lambda_\beta}; P_\beta = 1 - P_\alpha = \frac{\Lambda_\beta}{\Lambda_\alpha + \Lambda_\beta}; \lambda_{\alpha,i} = \Lambda_\alpha \log\left(\frac{1}{\xi}\right)$$

$$\Lambda_C = \frac{\Lambda_\alpha \Lambda_\beta}{\Lambda_\alpha + \Lambda_\beta}; \quad I = \frac{r}{\Lambda_C}; \quad f(k, I) = e^{-I}\frac{(I)^k}{k!}$$



Randomly place interfaces in domain.



Other Methods for Transport in Stochastic Media

- **Benchmark (brute force)**
  - Transport on each ensemble of realizations
  - Exact if can sample random media, but show to converge
- **Atomic Mix Approximation (AM)**
  - Assuming mixing at atomic level (autocorrelation=0)
  - Exact in diffusive limit
- **Chord Length Sampling (CLS/Algorithm A)**
  - Levermore-Pomraning Closure MC Equivalent
  - Exact for purely absorbing
  - No material memory

G. B. ZIMMERMAN and M. L. ADAMS, "Algorithms for Monte-Carlo Particle Transport in Binary Statistical Mixtures," *Trans. Am. Nucl. Soc.*, **63**, 287 (1991).

P. S. BRANTLEY and G. B. ZIMMERMAN, "Benchmark comparison of Monte Carlo algorithms for three-dimensional binary stochastic media," *Trans. Am. Nucl. Soc.*, **117**, 765–768 (2017).

- **Local Realization Preserving (LRP/Algorithm B)**
  - Some material memory
- **Algorithm C**
  - Even more material memory

Outline

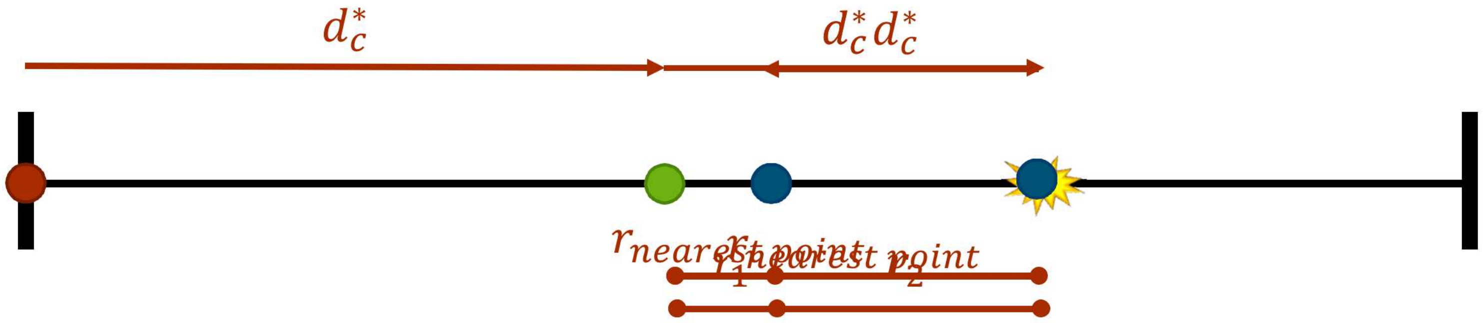
- Introduction and Problem Statement
- **Example Use of Conditional Point Sampling Approach**
- Conditional Point Sampling Analysis
- Conclusion and Future Work

Conditional Point Sampling: Animation of Algorithm

Material α

Material β

Particle



$\mu = \cos\theta$

$d_b = domain$

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

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

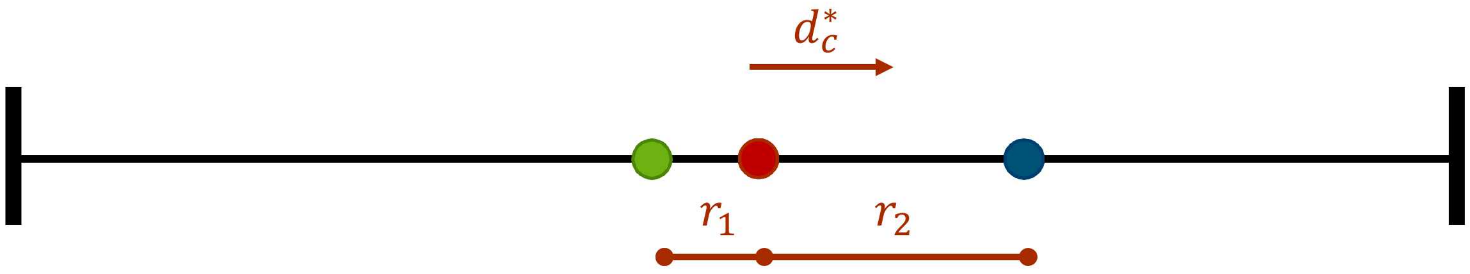
$P_{col} = \frac{\Sigma_t}{\Sigma_t^*}$

CoPS

1. Begin Woodcock Monte Carlo Algorithm.
   - Initialize x and μ.
2. Sample distance to ***potential*** collision, d_c^*, and distance to boundary, d_b.
3. Stream particle based on, $d_{min} = min(d_c^*, d_b)$.
   - If external boundary is crossed, terminate particle.
   - If particle streams to potential collision site, sample material at that point using P_α or $conditional\ probability\ function$.
4. Sample against P_{col} to determine if collision is accepted.
   - If collision is rejected, continue streaming particle by returning to step 2.
   - If collision is accepted, evaluate collision.

Conditional Point Sampling: Algorithm

Material α
Material β



$\mu = \cos\theta$

$d_b = domain$

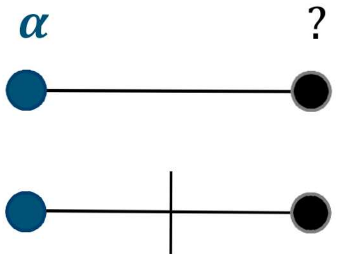
$d_c^* = -\frac{1}{\Sigma_t^*}\log(\xi)$

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

$P_{col} = \frac{\Sigma_t}{\Sigma_t^*}$

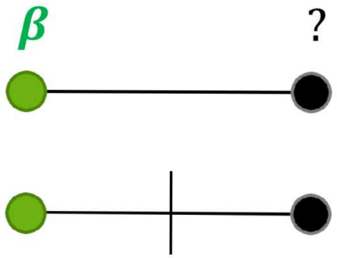
1. Begin Woodcock Monte Carlo Algorithm.
    - Initialize x and μ.
2. Sample distance to ***potential*** collision, d_c^*, and distance to boundary, d_b.
3. Stream particle based on, $d_{min} = min(d_c^*, d_b)$.
    - If external boundary is crossed, terminate particle.
    - If particle streams to potential collision site, sample material at that point using P_α or $conditional\ probability\ function$.
4. Sample against P_{col} to determine if collision is accepted.
    - If collision is rejected, continue streaming particle by returning to step 2.
    - If collision is accepted, evaluate collision.

Conditional Point Sampling: Deriving 2-Point Conditional Probability Function



$$\pi(m=\alpha|\boldsymbol{m}=\alpha,\boldsymbol{r}=r_1)=(1)f(k=0,r=r_1)+(P_\alpha)f(k>0,r=r_1) \qquad (6a)$$

$$\pi(m=\alpha|\boldsymbol{m}=\alpha,\boldsymbol{r}=r_1)=1-(1-P_\alpha)\left(1-e^{-\frac{r_1}{\Lambda_c}}\right) \qquad (6b)$$

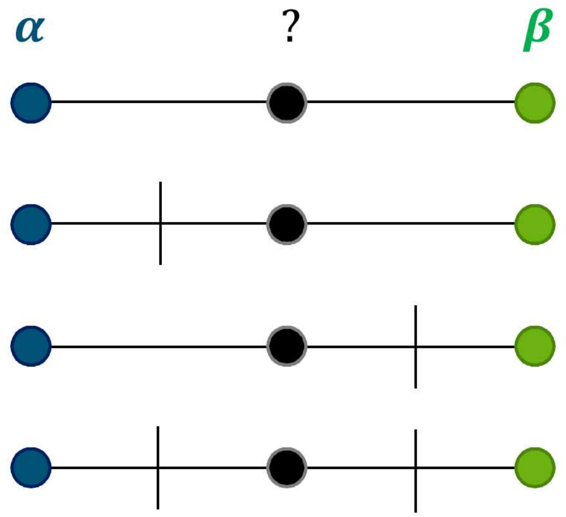


$$\pi(m=\alpha|\boldsymbol{m}=\beta,\boldsymbol{r}=r_1)=(0)f(k=0,r=r_1)+(P_\alpha)f(k>0,r=r_1) \qquad (7a)$$

$$\pi(m=\alpha|\boldsymbol{m}=\beta,\boldsymbol{r}=r_1)=P_\alpha\left(1-e^{-\frac{r_1}{\Lambda_c}}\right) \qquad (7b)$$

CoPS

Conditional Point Sampling: Deriving 3-Point Conditional Probability Function



$$\pi(m = \alpha | \boldsymbol{m} = \{\alpha, \beta\}, \boldsymbol{r} = \{r_1, r_2\}) = \Big[(0) f(k > 0, r = r_1) f(k = 0, r = r_2) + (1) f(k = 0, r = r_1) f(k > 0, r = r_2) + (P_\alpha) f(k > 0, r = r_1)\, f(k > 0, r = r_2) \Big] / (1 - f(k = 0, r = r_1 + r_2)) \quad (8)$$

$\pi(m = \alpha | \boldsymbol{m}, \boldsymbol{r})$

$\boldsymbol{m} = \{m_1, m_2\}$

$\boldsymbol{r} = \{r_1, r_2\}$

$$\pi(m = \alpha | \boldsymbol{m} = \{\alpha, \alpha\}, \boldsymbol{r} = \{r_1, r_2\}) = 1 - (1 - P_\alpha)\left(1 - e^{-\frac{r_1}{\Lambda_c}}\right)\left(1 - e^{-\frac{r_2}{\Lambda_c}}\right) \quad (9)$$

$$\pi(m = \alpha | \boldsymbol{m} = \{\beta, \beta\}, \boldsymbol{r} = \{r_1, r_2\}) = P_\alpha\left(1 - e^{-\frac{r_1}{\Lambda_c}}\right)\left(1 - e^{-\frac{r_2}{\Lambda_c}}\right) \quad (10)$$

$$\pi(m = \alpha | \boldsymbol{m} = \{\alpha, \beta\}, \boldsymbol{r} = \{r_1, r_2\}) = \frac{1}{1 - e^{-\frac{r_1 + r_2}{\Lambda_c}}} * \left(1 - e^{-\frac{r_2}{\Lambda_c}}\right)\left[1 - (1 - P_\alpha)\left(1 - e^{-\frac{r_1}{\Lambda_c}}\right)\right] \quad (11)$$

CoPS

Benchmark Suite Problem Parameters

- Adams Benchmark Suite Problem Parameters

Case Number	$\Sigma_{t,0}$	$\Sigma_{t,1}$	Λ_0	Λ_1
1	10/99	100/11	0.99	0.11
2	10/99	100/11	9.9	1.1
3	2/101	200/101	5.05	5.05

Case Letter	c_0	c_1	Slab Thickness	
a	0.0	1.0	$L =$	10.0
b	1.0	0.0		
c	0.9	0.9		

- $\Sigma_{t,j}$ – total cross section
- Λ_j – average chord length
- c_j – scattering cross section
- L – slab length
- $j \in \{0,1\}$ – material type

CoPS

Outline

- Introduction and Problem Statement
- Example Use of Conditional Point Sampling Approach
- **Conditional Point Sampling Analysis**
- Conclusion and Future Work

Results & Analysis: Leakage Results

- Reflectance and Transmittance Results for Slab Geometry $L = 10.0$

Case		Reflectance				Transmittance			
		Bench	Alg. C	CoPS2	CoPS3	Bench	Alg. C	CoPS2	CoPS3
1	a	0.4360(5)	0.4196(5)	0.4281(5)	0.4347(5)	0.0148(1)	0.0184(1)	0.0163(1)	0.0147(1)
	b	0.0850(2)	0.0812(2)	0.0747(2)	0.0845(2)	0.00166(4)	0.00161(4)	0.00162(5)	0.00161(5)
	c	0.4777(4)	0.4364(4)	0.4514(4)	0.4720(4)	0.0163(1)	0.0179(1)	0.0167(1)	0.0159(1)
2	a	0.2372(4)	0.2365(4)	0.2338(4)	0.2374(4)	0.0980(2)	0.0990(2)	0.1001(3)	0.0982(2)
	b	0.2876(4)	0.2877(4)	0.2605(4)	0.2861(4)	0.1952(3)	0.1951(3)	0.1898(3)	0.1957(3)
	c	0.4326(4)	0.4303(4)	0.4072(4)	0.4331(4)	0.1870(3)	0.1864(3)	0.1904(3)	0.1870(3)
3	a	0.6904(4)	0.6872(4)	0.6824(4)	0.6903(4)	0.1639(3)	0.1672(3)	0.1723(3)	0.1644(3)
	b	0.0363(1)	0.0363(1)	0.0310(1)	0.0359(1)	0.0762(2)	0.0763(2)	0.0761(2)	0.0763(2)
	c	0.4451(4)	0.4409(4)	0.4212(4)	0.4435(4)	0.1042(3)	0.1041(3)	0.1067(3)	0.1040(3)

CoPS

Calculating Error Metrics

- Relative Error

$$E_{R_i} = \frac{x_{approx_i} - x_i}{x_i}, \qquad i \in \{1a, 1b, 1c, 2a, 2b, 2c, 3a, 3b, 3c\} \tag{14}$$

- Root Mean Squared Error

$$RMS\ E_R = \sqrt{\frac{1}{N} \sum_i {E_R}_i^2} \tag{15}$$

- Average Absolute Error

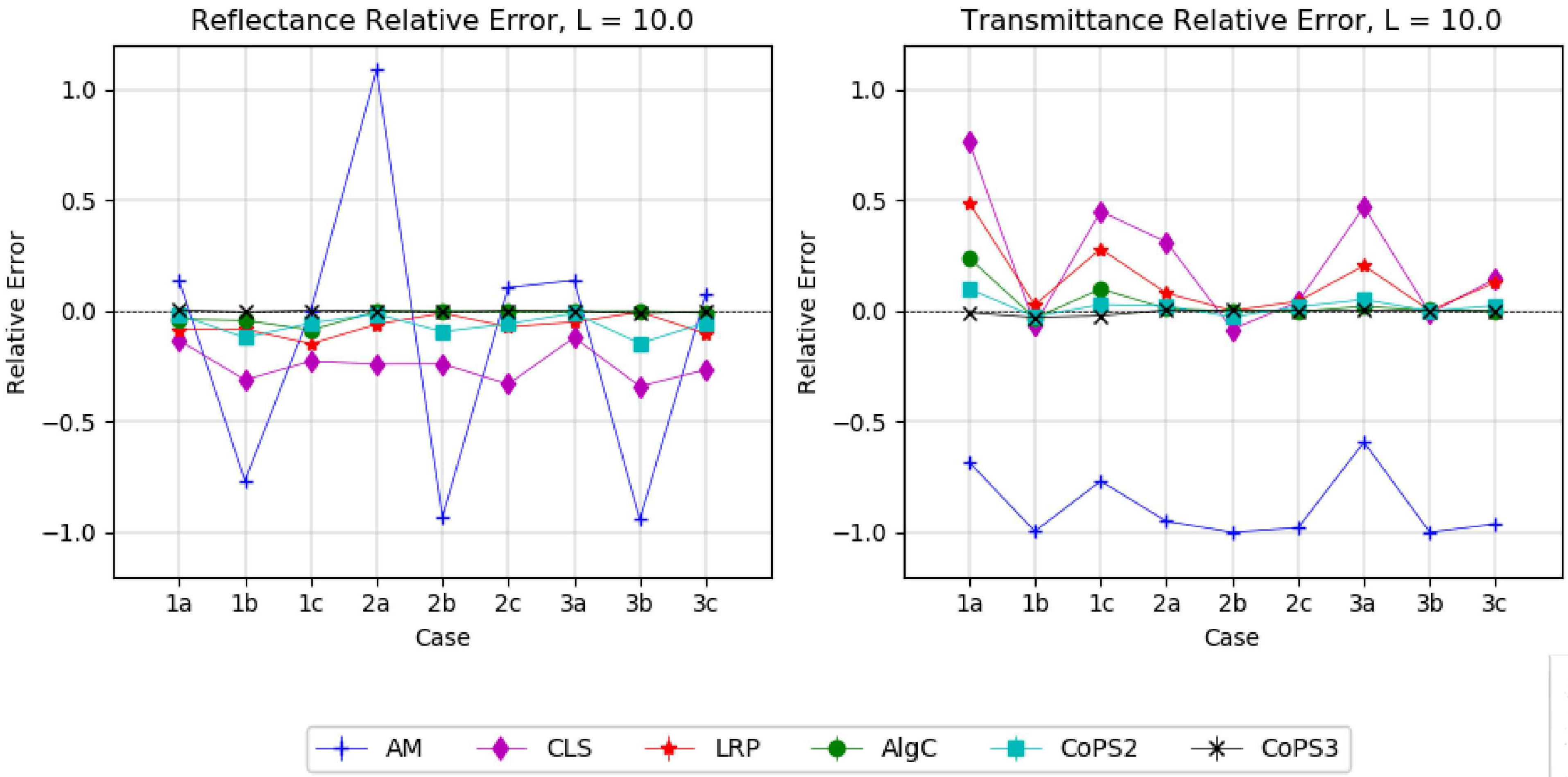
$$Mean\ |\mathrm{E}_R| = \frac{1}{N} \sum_i |E_{R_i}| \tag{16}$$

- Maximum Absolute Error

$$Max\ |\mathrm{E}_R| = \max |{E_R}_i| \tag{17}$$

CoPS

Results & Analysis: Leakage Relative Error



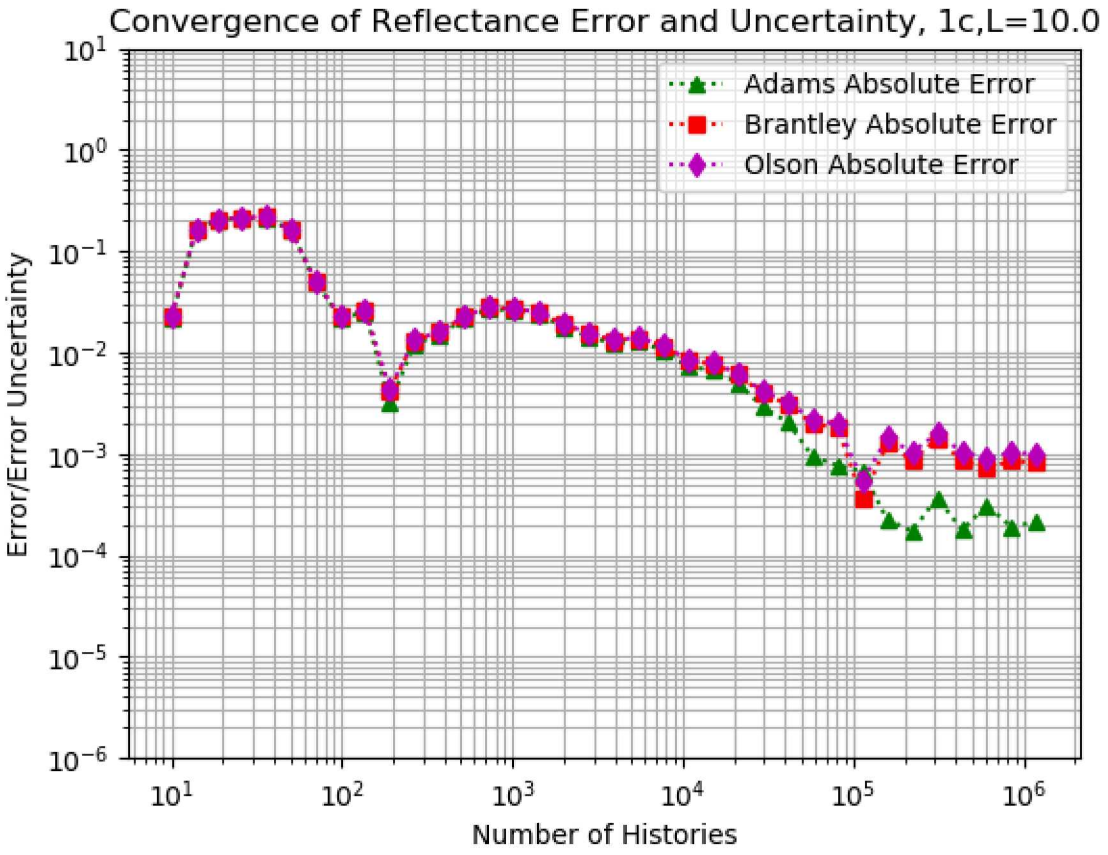
Results & Analysis: Solver Error

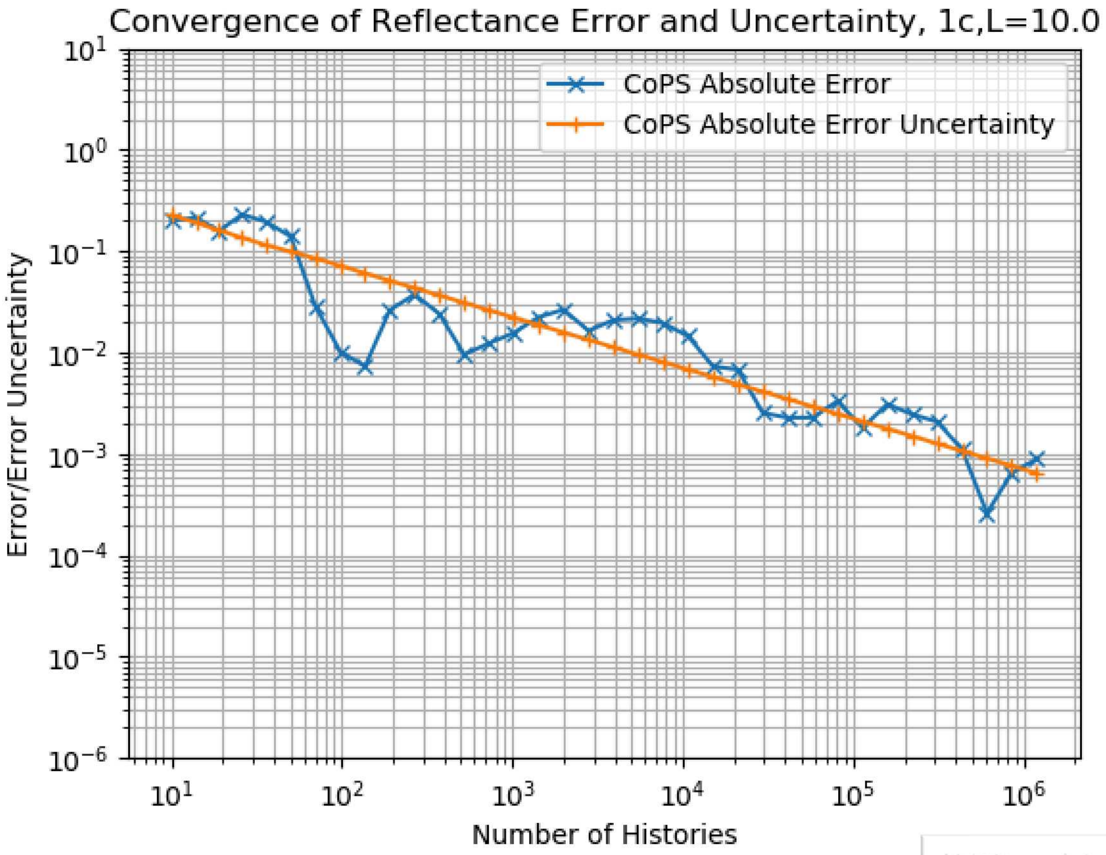
- Reflectance and Transmittance Metrics for Relative Error Over Cases

Leakage	Error	AM	CLS	LRP	Alg. C	CoPS2	CoPS3
Ref.	RMS E_R	0.631	0.257	0.080	0.035	0.078	0.005
	Mean $\|E_R\|$	0.465	0.246	0.069	0.021	0.064	0.003
	Max $\|E_R\|$	1.088	0.341	0.148	0.087	0.146	0.011
Trans.	RMS E_R	0.894	0.355	0.207	0.087	0.042	0.013
	Mean $\|E_R\|$	0.881	0.260	0.139	0.045	0.033	0.008
	Max $\|E_R\|$	1.000	0.765	0.489	0.239	0.099	0.030

CoPS

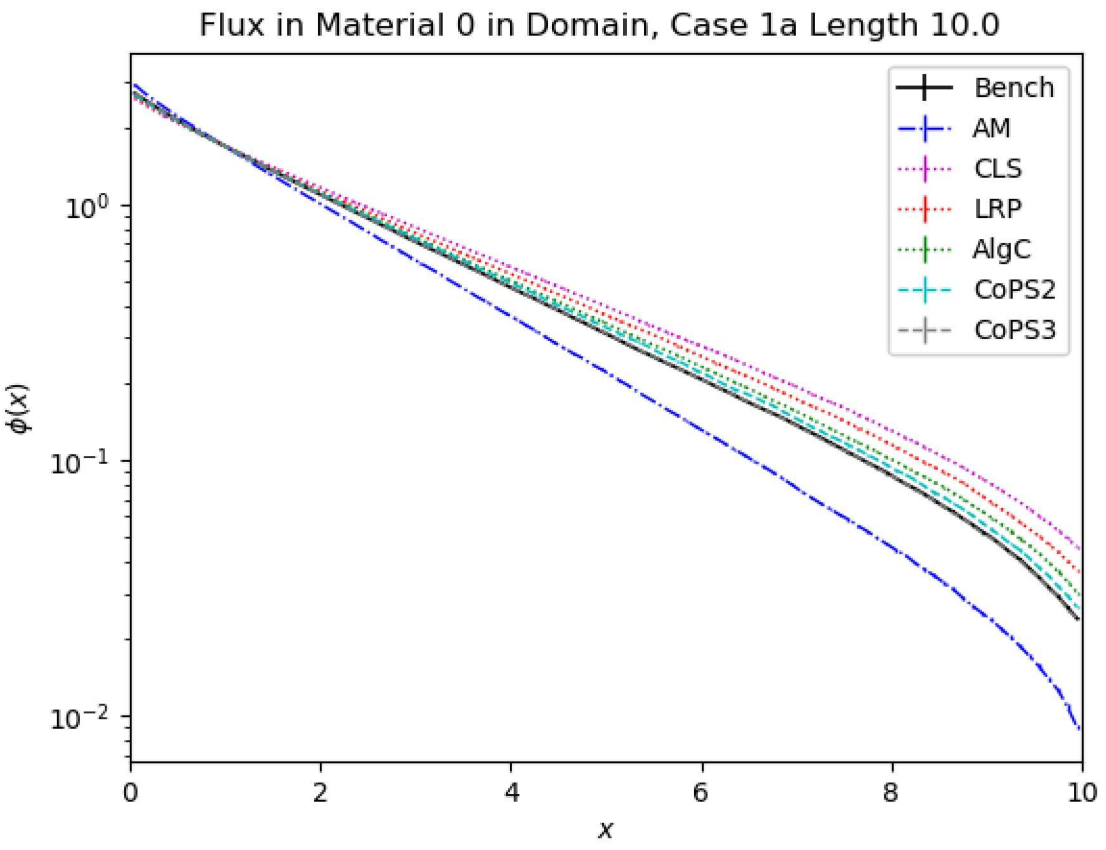
Results & Analysis: Convergence Study

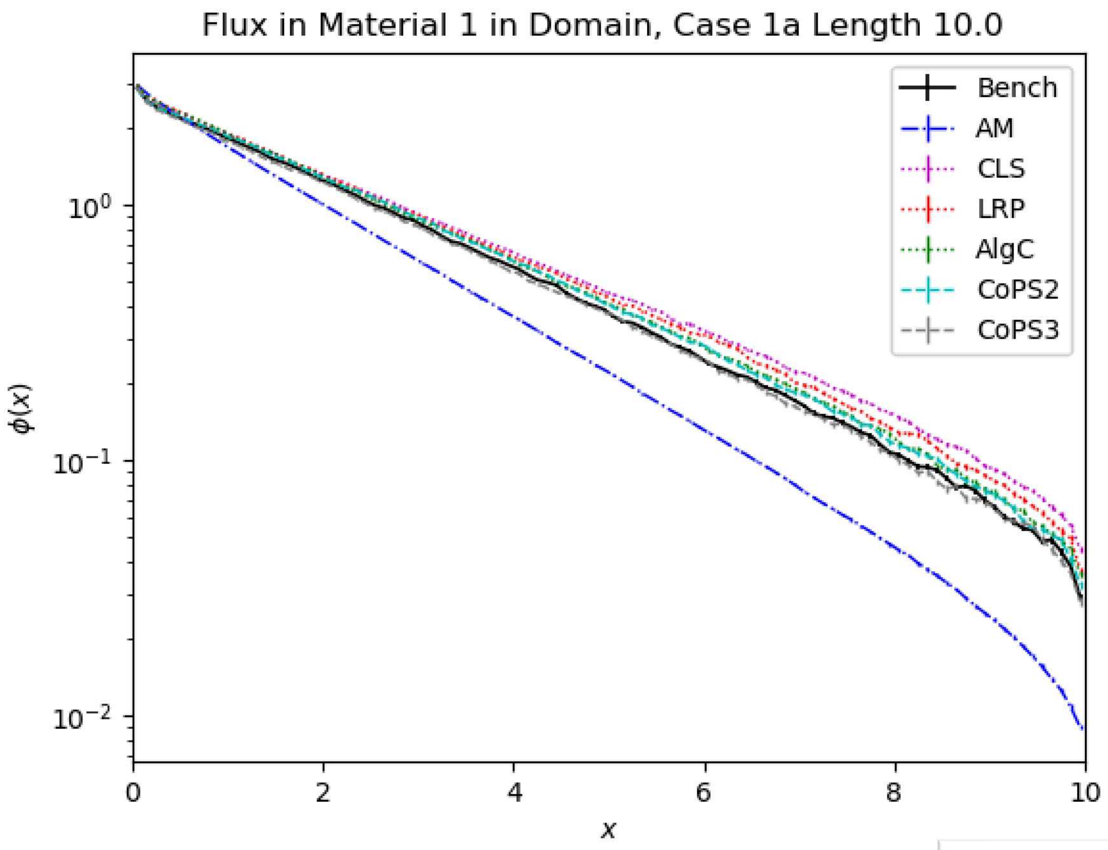




CoPS

Results & Analysis: Flux Tallies





Outline

- Introduction and Problem Statement
- Example Use of Conditional Point Sampling Approach
- Conditional Point Sampling Analysis
- **Conclusion and Future Work**

CoPS

Conclusion

- Provided numerical Alg. C leakage values
- CoPS algorithm is demonstrated yielding leakage, material-independent, and material-dependent flux values.
- CoPS2 performed as well as LRP for reflectance values and better than Alg. C for transmittance values.
- Conducted convergence studies to demonstrate that CoPS3 produced the most accurate results with no bias error for 1D Markovian-mixed media.

Future Work

Completed Work

- Calculate spread of results due to material mixing
- Multi-dimensions

Future Work

- Multi-material
- Non-Markovian-mixed Media
- Investigate CoPS efficiency
- Investigate implementation of biased Woodcock tracking

Acknowledgements

- Sandia National Laboratories
  - Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.
  - This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

- Internship Manager
  - Dr. Len Lorence
  - Dr. Joe Castro

- Internship Mentor
  - Dr. Aaron Olson

CoPS

CoPS

Questions?