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Radiation Transport in Random Media With Large Fluctuations

Aaron J. Olson,[*,†] Anil K. Prinja,[*] and Brian C. Franke[†]

[*]*Department of Nuclear Engineering, University of New Mexico, Albuquerque, NM 87131, USA*
[†]*Sandia National Laboratories, Albuquerque, NM 87185, USA*
aolson1@unm.edu, prinja@unm.edu, bcfrank@sandia.gov

INTRODUCTION

Strongly heterogeneous media arise in several applications that include radiation shields, nuclear fuel, BWR moderators, clouds, planetary and stellar atmospheres, turbulent gases and plasmas. Neutral and charged particle transport computations in such media have relied heavily on formulating transport equations with spatially random coefficients (physical data) and developing solution methods to deal with the additional stochastic dimensions. Attempts at developing approximate closures that yield only low order statistical information (e.g., mean and variance of the flux) have proved to be highly restrictive under real physics conditions [1, 2] or rely on techniques that require fluctuation amplitudes to be small for robustness [3]. Recently, stochastic spectral methods such as polynomial chaos and stochastic collocation [4] have been developed for aleatoric uncertainty quantification and sensitivity analysis, and successfully applied in radiation transport work [5, 6]. Advances in UQ techniques have tended to focus on efficiently handling large numbers of uncertain variables but the rigorous stochastic basis of the approach also promotes its use in situations where stochasticity is due to spatial heterogeneity and the associated uncertainty is large. Here we apply these techniques to radiation transport in media with spatially randomly varying cross sections without restriction on fluctuation amplitudes. Specifically, we represent the cross sections as a lognormal spatial random process with specified mean, variance and covariance function and use a Karhunen-Loève (KL) decomposition to generate cross section realizations that are strictly positive. Woodcock Monte Carlo (WMC) [7, 8, 9] is then used to simulate transport using random sampling of cross sections and deterministic sampling based on a stochastic collocation technique. Numerical results for the mean and variance in the scalar flux and leakage currents are obtained for weak and strong random variations. We focus in this work on demonstrating the approach and defer application to specific problems to a future investigation.

RANDOM TRANSPORT PROBLEM FORMULATION

The random transport equation of interest is given by

$$\mu\frac{\partial\psi(x,\mu,\omega)}{\partial x}+\sigma_t(x,\omega)\psi(x,\mu,\omega)=\frac{\sigma_s(x,\omega)}{2}\int_{-1}^{1}d\mu'\psi(x,\mu',\omega),$$
$$0\le x\le L;\qquad -1\le\mu\le 1$$
$$\psi(0,\mu,\omega)=\delta(1-\mu),\quad \mu>0;\qquad \psi(s,\mu,\omega)=0,\quad \mu<0, \tag{1}$$

where the label ω denotes a particular realization of the spatially random scattering $\sigma_s(x,\omega)$ and absorption $\sigma_a(x,\omega)$ cross sections but otherwise standard notation has been used. The successful solution of this problem depends upon (i) the ability to efficiently construct individual realizations of the random physical data, (ii) the existence of efficient numerical methods of solution for the transport equation, and (iii) postprocessing of the resulting random output to extract the quantities of physical interest. A random process that yields nonnegative spatial realizations of the cross sections and is widely employed in representing random physical properties characterized by large variances is the lognormal random process. In this representation, cross sections are expressed as

$$\sigma_r(x,\omega)=\exp[w_r(x,\omega)],\quad r=s,a, \tag{2}$$

where $w_r(x,\omega)$ is a Gaussian process with parameters chosen such that the correct mean, variance and covariance of the random cross sections are preserved. It is not difficult to show that the mean $\langle w_r\rangle$ and variance v_{w_r} of the Gaussian distribution are related to the mean $\langle\sigma_r\rangle$ and variance v_{σ_r} of the cross sections according to

$$\langle w_r\rangle=\ln\left(\frac{\langle\sigma_r\rangle^2}{\sqrt{v_{\sigma_r}+\langle\sigma_r\rangle^2}}\right);\quad v_{w_r}=\ln\left(\frac{v_{\sigma_r}}{\langle\sigma_r\rangle^2}+1\right). \tag{3}$$

It is also readily shown that the relative covariance of the Gaussian process $\rho_w(x,x')=C_w(x,x')/v_w$ can be explicitly obtained from the relative covariance of the cross section $\rho_\sigma(x,x')=C_\sigma(x,x')/v_\sigma$:

$$\rho_w(x,x')=\frac{\ln\left(\rho_\sigma(x,x')\frac{v_\sigma}{\langle\sigma\rangle}+1\right)}{\ln\left(\frac{v_\sigma}{\langle\sigma\rangle^2}+1\right)}. \tag{4}$$

The mean, variance and covariance completely characterize a Gaussian random process and realizations of Gaussian random processes can be easily generated from a stochastic spectral representation given by the Karhunen-Loève expansion:

$$w_r(x,\omega)=\langle w_r\rangle+\sqrt{v_{w_r}}\sum_{k_r=1}^{\infty}\sqrt{\gamma_{k_r}}\phi_{k_r}(x)\xi_{k_r}(\omega),\quad r=s,a. \tag{5}$$

Here, γ_k and $\phi_k(x)$ are eigenvalues and eigenfunctions of a homogeneous Fredholm integral equation of the second kind with kernel given by the covariance function and $\xi_k(\omega)$ are i.i.d. standard normal random variables [10]. The eigenvalues are all positive and ordered with decreasing magnitude, which makes computation feasible by truncation of the KL expansion at an order that captures most of the variability, depending on the strength of correlation [5, 10]. Also, the eigenspectrum can be obtained analytically for an exponential covariance (characterized by a correlation length λ_c), which is convenient for numerical work. If the covariance for the cross sections is exponential then it readily follows from Eq.(4) that the covariance for the Gaussian random process is nearly exponential for small correlation lengths $\lambda_{c,\sigma}/L$. For large $\lambda_{c,\sigma}/L$, the covariance approaches a linear (or triangular [10]) function. For the illustrative purposes of this work, we assume the Gaussian process covariance is exponential but obtain the associated correlation length by a least squares fit to the true Gaussian covariance that would be consistent with an exponential covariance for the cross sections. Figure 1 plots the actual covariance and for two values of v_{σ_r}, the true Gaussian process covariance, and best fit exponential ansatz.

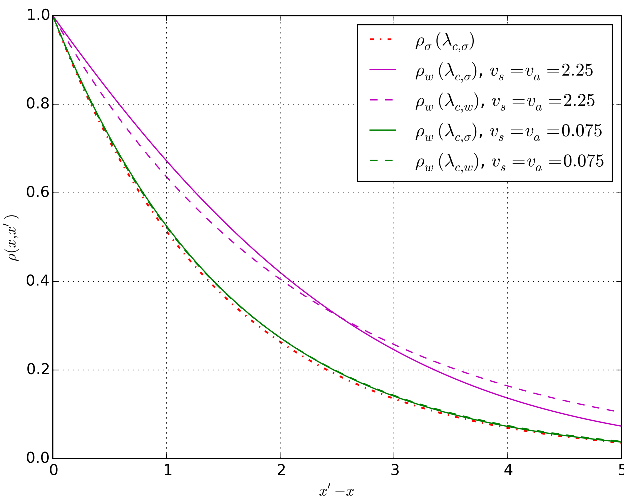

Fig. 1. Covariance Functions: Process ρ_σ, True Gaussian process $\rho_w(\lambda_{c,\sigma})$, Analytic Gaussian process $\rho_w(\lambda_{c,w})$

With the Gaussian process completely characterized and realizations of independent standard normal random variables readily sampled, realizations of cross sections are obtained from the truncated KL expression:

$$\sigma_r(x,\omega) = \exp\left[\langle w_r(x)\rangle + \sqrt{v_{w_r}} \sum_{k=1}^{K_r} \sqrt{\gamma_{k_r}}\phi_{k_r}(x)\xi_{k_r}(\omega)\right], \quad (6)$$

where we note that the number of eigenmodes K_r retained for the scattering and absorption cross sections need not be the same.

In Figure 2, fifty realizations of the lognormal cross section along with the mean and one and two standard deviation values are shown for a problem in which half of the ensemble average and variance is given to each constituent cross section. It is noted that the reconstructed cross sections are always positive and that many of the cross section values are clustered between zero and the mean but less frequently contain much higher values.

STOCHASTIC SAMPLING METHODS

In this work we are primarily interested in statistical averages of the flux (as well as leakage currents) which are defined with respect to the joint probability density $P(\xi_1,\ldots,\xi_N)$ over

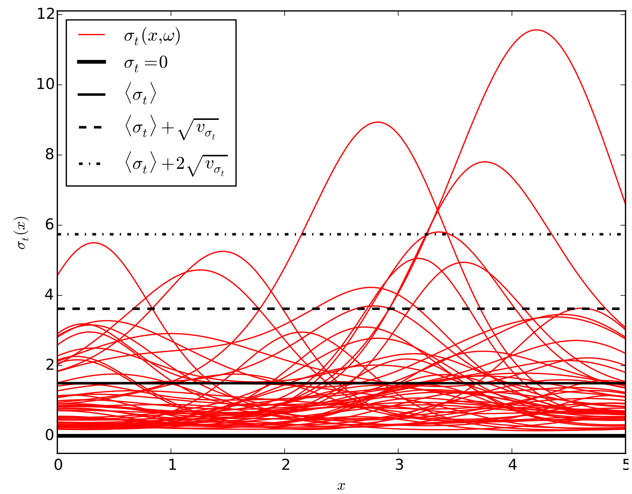

Fig. 2. Fifty Lognormal Realizations ($\langle\sigma_s\rangle = \langle\sigma_a\rangle = 0.75, v_{\sigma_s} = v_{\sigma_a} = 2.25$)

all random variables retained in the KL expansion as

$$\langle\phi^m\rangle = \int_{\xi_N}\cdots\int_{\xi_1}\phi^m(x,\xi_1,\ldots,\xi_N)P(\xi_1,\ldots,\xi_N)d\xi_1\cdots\xi_N, \quad (7)$$

and similarly for the leakage currents. In our case, the random variables are independent and the probability density factorizes into a product of standard normals for each random variable, i.e., $P(\xi_1,\ldots,\xi_N) = \prod_{n=1}^{N} P(\xi_n),\ \forall\ \xi_n \in N(0,1)$. We now describe two approaches to numerically evaluate Eq.(7).

In the first method, random sampling, or Monte Carlo (MC), is used to express the ensemble average as

$$\langle\phi^m\rangle \approx \frac{1}{R}\sum_{i=1}^{R}\phi^m(x,\xi_1^i,\ldots,\xi_N^i), \quad (8)$$

where R is the total number of realizations and ξ_n^i are values sampled from a standard normal distribution. We solve the transport equation in each realization, tallying moments of the flux and leakage values, then find the ensemble average expected value of the moments as the mean of these tallies. Random sampling in this manner converges the ensemble values as $R^{-0.5}$. This approach is dimensionally agnostic, meaning convergence is not affected by the number of random dimensions. We use random sampling with 10,000 realizations to generate a benchmark solution.

In the second method, Eq.(7) is numerically integrated by applying Gauss-Hermite quadrature over each variable. This so-called stochastic collocation (SC), or deterministic sampling, approach has the potential to produce accurate results with far fewer realizations than random sampling. KL random variable values $\xi_n^{q_n}$ are dictated by cubature node values, and averages are computed as

$$\langle\phi^m\rangle \approx \sum_{q_N}^{Q_N}\cdots\sum_{q_1}^{Q_1} w_{q_1}\cdots w_{q_N}\,\phi^m(x,\xi_1^{q_1},\ldots,\xi_N^{q_N}). \quad (9)$$

where w_{q_n} are the cubature weights. A direct approach uses an isotropic, full tensor product collocation grid over the random variables but requires $Q^{K_s+K_a}$ realizations, where Q is the quadrature order. Since the eigenvalues of the KL expansion monotonically decrease, it is straightforward to implement an anisotropic collocation grid, allocating a higher quadrature order to earlier and more weighty eigenmodes [11]. An anisotropic, full tensor product collocation grid requires solution of $\prod_{k_s}^{K_s} Q_{k_s} \cdot \prod_{k_a}^{K_a} Q_{k_a}$ realizations, where Q_{k_r} represents the quadrature order for eigenmode k_r for cross section r. Sparse collocation grids using Smolyak sparse grids would further allow dimensional reduction [5, 6, 11]. A more general approach would use sensitivity analysis [6] or adaptive collocation grids [6, 11] to choose optimal values for the number of KL eigenmodes kept and the quadrature order used in each dimension.

TRANSPORT RESULTS

Transport through each realization of the cross sections was effected using Woodcock Monte Carlo. This approach samples distance to collision according to the ceiling cross section in a particle flight path, then either accepts or rejects the collision, allowing transport calculations without cross section discretization in spatially continuously varying cross sections [7, 8]. Well chosen particle flight path domains, and thus ceiling cross sections, may serve to improve the efficiency of this method as a whole, and are a topic of future work. The underlying WMC transport solver has been benchmarked and utilized previously [9], and the new methods were benchmarked against uncollided flux calculations using a high order Gauss-Legendre quadrature to compute the optical depth of lognormal random processes.

Figures 3 and 4 show results for the mean, standard deviation, and relative standard deviation of the scalar flux in the medium for a very large relative variance problem with parameters $\langle\sigma_s\rangle = \langle\sigma_a\rangle = 0.75$, $v_{\sigma_s} = v_{\sigma_a} = 2.25$, $\lambda_{c,\sigma} = 1.5$, and $L = 5.0$. Results are shown for the following models: (i) zero variance or atomic mix (AM), (ii) random sampling Monte Carlo, (iii) isotropic stochastic collocation (iSC) grid, and (iv) anisotropic stochastic collocation (aSC) grid. In all cases the exponential ansatz with a best-fit $\lambda_{c,w}$ for the Gaussian covariance function was used. The random sampling Monte Carlo simulation used 10,000 realizations and KL truncation parameters $K_s = K_a = 4$. The isotropic SC approach uses quadrature order $Q = 3$ and $K_s = K_a = 4$, for a total of 6561 realizations. The anisotropic SC approach uses KL truncation $K_s = 4$ with quadrature orders $Q_{k_s} = \{4, 3, 3, 2\}$ and KL truncation $K_a = 3$ with quadrature orders $Q_{k_a} = \{4, 3, 2\}$, for a total of 1728 realizations. In all cases, 100,000 particle histories were simulated in each realization using Woodcock Monte Carlo. In Figure 5 these results are contrasted against a low variance medium, with $v_{\sigma_s} = v_{\sigma_a} = 0.075$.

The results show that cross section fluctuations cause deeper penetration of particles, an effect that is strongly correlated with the fluctuation amplitude or variance. With increasing variance, realizations with cross section values significantly less than the mean apparently increasingly dominate the transport, although the effect undoubtedly depends on other parameters held fixed in the present simulations. The atomic mix result is only reasonable for very small amplitude fluctuations and, in the problem investigated here, near the left boundary where the influence of the deterministic source is significant. These plots and the results for the transmittance and reflectance shown in Tables I and II confirm that high accuracy is possible with the stochastic collocation method at significantly reduced cost compared to random sampling. Further refinement of the anisotropic grid formulation, such as incorporating sparse grids with adaptivity, will yield greater efficiency and make feasible the solution of large variance problems with high stochastic dimensionality.

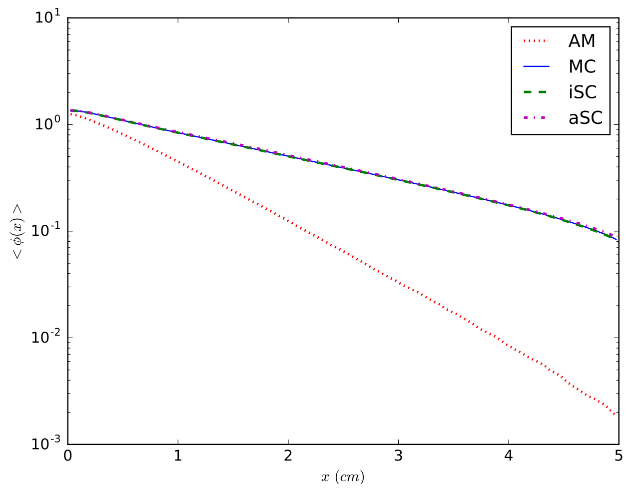

Fig. 3. Mean Scalar Flux in Slab

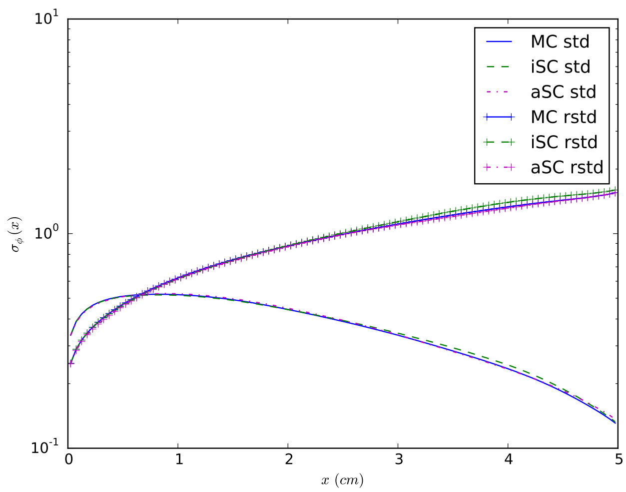

Fig. 4. Standard Deviation (std) and Relative Standard Deviation (rstd) of Scalar Flux in Slab

CONCLUSIONS

We have demonstrated that a combination of stochastic spectral representation and Woodcock Monte Carlo simulation allows efficient computation of radiation transport in strongly random media. The use of a lognormal distribution to represent the fluctuations in medium properties facilitates enforcement of strict positivity of cross section realizations, a condition that has challenged standard approaches that assume

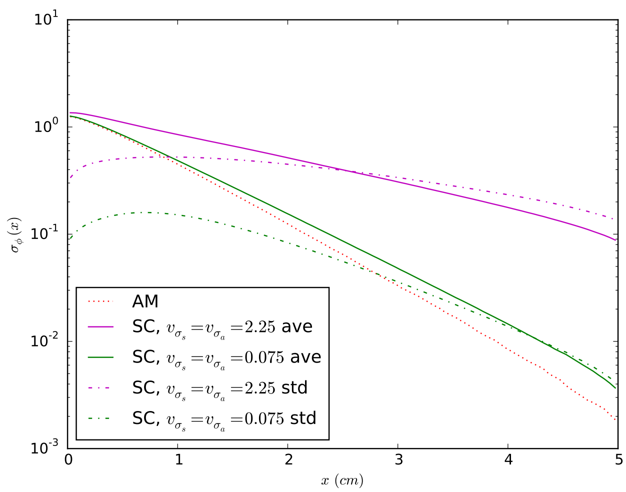

Fig. 5. AM and Anisotropic SC Flux Average and Standard Deviation Profiles

TABLE I. Transmittance Values

	average	deviation	SEM
AM	0.00131		
MC, $v_{\sigma_s} = v_{\sigma_a} = 2.25$	0.06221	0.09862	0.00099
iSC, $v_{\sigma_s} = v_{\sigma_a} = 2.25$	0.06074	0.09844	
aSC, $v_{\sigma_s} = v_{\sigma_a} = 2.25$	0.06640	0.10438	
aSC, $v_{\sigma_s} = v_{\sigma_a} = 0.075$	0.00262	0.00294	

TABLE II. Reflectance Values

	average	deviation	SEM
AM	0.11442		
MC, $v_{\sigma_s} = v_{\sigma_a} = 2.25$	0.16254	0.14528	0.00145
iSC, $v_{\sigma_s} = v_{\sigma_a} = 2.25$	0.16228	0.14471	
aSC, $v_{\sigma_s} = v_{\sigma_a} = 2.25$	0.16474	0.14665	
aSC, $v_{\sigma_s} = v_{\sigma_a} = 0.075$	0.12007	0.03840	

Gaussian fluctuations. The fact that the lognormal random process is a memoryless nonlinear transformation of a Gaussian process further enables efficient and accurate reconstruction of the random cross section realizations using a Karhunen-Loève representation of the cross section. Finally, the robustness of this model enables fluctuations of arbitrarily large amplitude to be studied, using both random sampling Monte Carlo and more efficient stochastic collocation techniques. The present work is being extended to allow reconstruction of probability density functions of output variables using polynomial chaos representation, and to accommodate general cross section covariance functions. Also, techniques are being explored to more judiciously select ceiling cross sections to enhance the efficiency of Woodcock Monte Carlo for transport in random media.

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