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STOCHASTIC AVERAGING OF CROSS SECTION UNCERTAINTY IN RADIATION TRANSPORT

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ABSTRACT

Radiation transport in a one dimensional random medium is considered. The Karhunen-Loève spectral expansion method is shown to provide an efficient representation of the total cross section that is a continuous random process in space. Numerical results for an exponential covariance function show that a low order truncation suffices to capture the dominant components of the random process for reasonable choices of physical parameters. For Gaussian statistics, Gauss-Hermite quadrature is used to compute the mean scalar flux, with acceptable convergence to the exact result possible with relatively low expansion and quadrature orders. For scattering dominated optically thick, large fluctuation problems, the numerical results show that the random transport equation is accurately approximated by a nonrandom diffusion equation with a diffusion equation determined solely by the mean cross section.

Key Words: random medium transport, Karhunen-Loève expansion, quadrature averaging

1. INTRODUCTION

We describe a computationally efficient closure-free method for quantifying the effect of cross section uncertainty in the the numerical solution of the transport equation. The origin of the uncertainty can be physical, such as random mixtures of immiscible materials [2], or it can represent limitations in the accuracy of measurements of physical properties. The assumption of this work is that physical property uncertainty can be described in the language of random processes and is statistically sufficiently well-characterized through relevant probability distribution functions or moments and correlation functions. The problem then becomes one of radiation transport in random media and the specific goal is to obtain reduced-order transport models for the statistical moments or ensemble averages of the angular flux and other physical quantities of interest (such as dose).

Ensemble averages of the angular flux can be obtained in principle by numerically solving the transport equation, using standard deterministic or stochastic methods, for a statistically significant number of realizations of the cross section. However, this Monte Carlo approach is generally impractical because of the well known slow convergence of direct sampling methods which requires that the transport equation be solved for an inordinately large number of realizations. For spatially continuous random cross sections, this inefficiency is compounded by the need to span a dense sample space of cross section realizations. Consequently, solutions generated in this way are typically used only for assessing the accuracy of approximation methods, but as this is obviously an important requirement, it is necessary that methods for direct numerical solution be available, even if they are expensive to implement. At the other extreme, closure methods [1, 2] seek to obtain a small number of deterministic transport-like equations directly for ensemble averages, which makes this approach computationally very attractive. However, closures tend to

be highly specialized, their predictive capability deteriorates rapidly outside their domain of strict validity and they do not lend themselves to generalization.

The motivation behind the present work was to investigate a method that has the potential of being orders of magnitude faster computationally than sampling methods and which has broader applicability than closure approximations. Our approach to transport in random media combines two elements to try to achieve computational efficiency. First, it is based on a spectral expansion of the random cross section in terms of a unique basis in the Hilbert space of second-order random processes. This representation is given by the Karhunen-Loève (KL-) expansion [3, 4], which is an optimal expansion in eigenmodes of the covariance function associated with the random process. A unique feature of this representation is that it can be truncated at a low order for typical physically valid cross section parameter choices. This has the effect that a complicated random process can be characterized by a small number of uncorrelated random variables and makes possible the second step in our scheme, namely, the use of quadratures in lieu of realization averaging of the transport equation. We demonstrate this methodology specifically for the cross section described by a Gaussian stochastic process and show numerical results for the mean scalar flux as well as scalar flux realizations as a function of the random and nonrandom parameters in the problem. Also, the use of a Gaussian model of fluctuations makes possible an exact closure of the ensemble averaged transport equation [6] and this result is used as a benchmark.

The scope of the paper is as follows. The transport problem is defined in the next section which also includes a discussion of the random cross section. The Karhunen-Loève spectral expansion is then discussed in detail in the following section after which the numerical solution of the random transport equation is described. Numerical results are then presented and the paper closes with some concluding remarks.

2. TRANSPORT MODEL WITH RANDOM CROSS SECTION

We consider steady state particle transport in a subcritical one dimensional slab of thickness l_x with a spatially random total cross section. The specific transport problem is defined by:

$$\mu\frac{\partial\Psi(x,\mu,\omega)}{\partial x}+\Sigma(x,\omega)\Psi(x,\mu,\omega)=c\frac{\Sigma(x,\omega)}{2}\int_{-1}^{1}d\mu'\Psi(x,\mu',\omega)+\frac{Q}{2},$$
$$0\le x\le l_x,\ -1\le\mu\le 1, \tag{1}$$

$$\Psi(0,\mu,\omega)=0,\ \mu>0, \tag{2}$$
$$\Psi(l_x,\mu,\omega)=0,\ \mu<0. \tag{3}$$

The random total cross section $\Sigma(x,\omega)$ is a continuous deterministic function of position x for each realization, denoted by the symbol ω (also referred to as the random dimension), drawn from a sample space of realizations Ω. The mean number of secondaries $0<c<1$ is taken to be a deterministic quantity. In other words, we are assuming that the randomness in the macroscopic cross section is expressed solely through fluctuations in the atomic density: $\Sigma_{a,s}(x,\omega)=N(x,\omega)\,\sigma_{a,s}$. This is not a limitation of the approach used here, which can in fact handle quite general types of randomness. The restriction allows us to focus on the essential elements of the methodology but it also enables an exactly closed equation for the ensemble averaged flux to be obtained under certain conditions and therefore provides an important benchmark for the numerical simulations. A uniformly distributed nonrandom source is assumed for

illustration, but again this is not strictly necessary as the methodology can accommodate spatially random sources as well. Finally, the angular flux $\Psi(x,\mu,\omega)$ and scalar flux $\Phi(x,\omega) = \int_{-1}^{1} d\mu'\, \Psi(x,\mu',\omega)$ are also random functions in that for fixed phase space coordinates (x,μ), they have different values for different realizations of the cross section.

A key problem in the numerical solution of physical problems when the physical data are continuous random processes is the numerical representation of such random processes. This becomes clear if we recall the definition of a random process as an indexed random variable, i.e., a random variable with a (real) parameter. Our random cross section can then be viewed as a random variable for each value of the spatial index x, but since x ranges over a continuum of values, the cross section is in fact an *infinite dimensional* random variable. Expressed differently, while a random variable is completely defined by its one-point probability density function $P(\Sigma)d\Sigma$, the complete characterization of a random process requires knowledge of the infinite hierarchy of multi-point probability density functions given by $P(\Sigma_1,x_1)d\Sigma_1$, $P_2(\Sigma_1,x_1;\Sigma_2,x_2)d\Sigma_1 d\Sigma_2, \cdots \lim_{n\to\infty} P_n(\Sigma_1,x_1;\Sigma_2,x_2;\cdots\Sigma_n,x_n)d\Sigma_1\, d\Sigma_2\, \cdots d\Sigma_n$. For practical purposes, it is then necessary to construct a discretization of the stochastic dimension where the infinite dimensional process is replaced by a finite set of random variables. If this set is sufficiently small, and if the statistical properties of the reduced-dimension random variables can be characterized, a number of techniques for numerical solution of random transport equations become feasible, besides direct sampling Monte Carlo. For instance, quadrature-based methods can be used to obtain averages of the angular flux, an approach that is known to be very effective when the random dimension is small. Alternatively, the angular flux can be expanded in random orthogonal basis functions (such as multi-dimensional random Hermite polynomials). Using an appropriate inner product, a Galerkin projection technique can then be used to generate a set of coupled *deterministic* transport equations for the expansion coefficients. This so-called stochastic finite element method has found widespread and successful implementation in structural mechanics [3] but remains relatively unexplored territory in radiation transport applications. However, this approach becomes computationally demanding if a significant number of random variables need to be retained.

The purpose of this work is threefold. First, we describe a well-known, optimal modal decomposition of the random cross section and numerically demonstrate its dimension-reducing features. Second, for a specific statistical model of cross section fluctuations, we combine quadrature averaging with a discrete ordinates, finite element numerical solution of the reduced order transport equation to show the efficacy of this spectral representation. Third, we present numerical results that show very interesting behavior in scalar flux realizations as the medium is made optically thick.

3. SPECTRAL REPRESENTATION OF THE CROSS SECTION: THE KARHUNEN-LOÈVE EXPANSION

Before proceeding with the spectral decomposition, we first establish notation and some technical conditions on the type of random processes that can be accommodated by this methodolody [3–5]. Ensemble averages will be defined in terms of the mathematical expectation with respect to an appropriate probability measure. Thus, the mean cross section is expressed as

$$\langle\Sigma\rangle(x) = E[\Sigma] = \int_0^\infty \Sigma\, P(\Sigma,x)d\Sigma, \tag{4}$$

and the variance as

$$\langle\tilde{\Sigma}^2\rangle(x) = \langle(\Sigma - \langle\Sigma\rangle)^2\rangle = E[(\Sigma - \langle\Sigma\rangle)^2] = \int_0^\infty (\Sigma - \langle\Sigma\rangle)^2\, P(\Sigma,x)d\Sigma. \tag{5}$$

In developing finite dimensional representations of continuous random processes we specialize to second-order random processes. A second-order random variable Σ is a random variable with a finite mean-square value, $E[\Sigma^2] < \infty$, and hence a finite variance. A second-order random process $\Sigma(x)$ is a second-order random variable for each value of x. It has a finite covariance defined by,

$$\begin{aligned} C_\Sigma(x,x') &= E\left[(\Sigma(x) - \langle\Sigma\rangle(x))\ (\Sigma(x') - \langle\Sigma\rangle(x'))\right] \\ &= \iint (\Sigma - \langle\Sigma\rangle(x))\,(\Sigma' - \langle\Sigma\rangle(x')\,P(\Sigma,x;\Sigma',x')d\Sigma\,d\Sigma' < \infty. \end{aligned} \tag{6}$$

In particular, the variance of a second-order random process is finite: $\langle\tilde{\Sigma}^2\rangle(x) = C(x,x) < \infty$. We also require the second order random process to be continuous is quadratic mean (q.m. continuous): a second order process is q.m. continuous if $\lim_{h\to 0} E[(\Sigma(x+h) - \Sigma(x))^2] = 0$, $x \in [0, l_x]$. This condition ensures continuity of the covariance function $C_\Sigma(x,x')$ on the square $l_x \times l_x$, which plays a central role in the spectral expansion to be presented below. We comment parenthetically that since the randomness presumably arises from physical processes, the assumption of a second order q.m. continuous random cross section does not represent a limitation. The following well-established results from the theory of second-order random processes will be relevant [5]. The vector space of realizations of the cross section is an infinite dimensional Hilbert space with inner product $< \Sigma|\Sigma' >$ given by the expectation $E[\Sigma\,\Sigma']$ and norm $||\Sigma||_2 = \sqrt{E[\Sigma^2]}$. Any complete, countable orthonormal set in the Hilbert space will be an orthonormal basis and every element (every cross section realization, in our context) can be expanded in terms of the basis vectors. This representation will be a generalized Fourier series expansion of the type:

$$\Sigma(x,\omega) = \sum_{n=1}^{\infty} a_n(\omega)\,\phi_n(x), \tag{7}$$

where $\{\phi_n\}$ are the basis vectors defined on the (finite) support of x and $\{a_n(\omega)\}$ are random expansion coefficients. The implied convergence in Eq.(7) is understood to be in q.m. sense:

$$\lim_{N\to\infty} E\left[\left(\Sigma(x,\omega) - \sum_{n=1}^{N} a_n(\omega)\,\phi_n(x)\right)^2\right] = 0, \quad \text{uniformly in } x. \tag{8}$$

Since the expansion coefficients $a_n(\omega)$ are constants, Eq.(7) is a representation of a random process in terms of a countably infinite set of random variables. This representation remains computationally intractable, however, because of the infinity of terms required, but, with an appropriate choice of basis, finite-dimensional subspaces can be considered which best capture the dominant features of the randomness. That is, a carefully constructed basis would enable the expansion in Eq.(7) to be truncated at a low order and provide the desired discretization of the random process. A complete set of orthonormal basis vectors can be broadly selected from elementary square-integrable functions, the most familiar being the sinusoidal functions from classical spectral theory. However, it turns out that this is not the most efficient choice of basis because it is constructed independently of the random structure in the physical data.

The optimal representation is provided by the Karhunen-Loève (K-L) expansion [3, 4] which is based on the eigen-decomposition of the covariance function $C_\Sigma(x,x')$. The covariance is a continuous, real, symmetric and positive definite function on $[0,l_x] \times [0,l_x]$ and, according to Mercer's theorem [5], it has the spectral decomposition:

$$C_\Sigma(x,x') = \sum_{n=0}^{\infty} \lambda_n \phi_n(x)\phi_n(x') \tag{9}$$

where $\{\phi_n,\ \lambda_n\}$ are the eigenfunctions and eigenvalues of the following self-adjoint Fredholm integral equation with the covariance function as the kernel:

$$\int_0^{l_x} C_\Sigma(x,x')\,\phi_n(x')\,dx' = \lambda_n\,\phi_n(x). \tag{10}$$

The following properties can be established [3–5]:

- The eigenfunctions ϕ_n are orthogonal with respect to the usual inner product in $L_2[0,l_x]$, they form a complete set, and can be normalized, i.e.,

$$\langle\phi_n|\phi_k\rangle = \int_0^{l_x} \phi_n(x)\phi_k(x)dx = \delta_{kn}. \tag{11}$$

- The eigenvalues λ_n are real, positive and countably infinite, and can be ordered according to $\lambda_1 > \lambda_2 > \lambda_3 \ldots$.

The significance of the above result is the following: for $\Sigma(x,\omega)$ a q.m. continuous second-order random process with covariance $C_\Sigma(x,x')$, the Karhunen-Loève expansion theorem [3] shows that that Σ can be expressed as

$$\Sigma(x,\omega) = \langle\Sigma\rangle + \sum_{k=1}^{\infty} \sqrt{\lambda_k}\,\phi_k(x)\,\xi_k(\omega), \tag{12}$$

where the mean cross section has been isolated so that the modal expansion is performed on the fluctuating component $\tilde{\Sigma}(x,\omega) = \Sigma(x,\omega) - \langle\Sigma\rangle$. Here, $\{\phi_n,\ \lambda_n\}$ are as defined above in the spectral decomposition of the covariance function and, importantly, the Fourier coefficients $\xi_k(\omega)$ are zero mean, uncorrelated random variables with unit variance, i.e.,

$$\langle\xi_k\rangle = 0, \tag{13}$$

$$\langle\xi_k\,\xi_l\rangle = \delta_{kl}. \tag{14}$$

This expansion is called the Karhunen-Loève (KL-) expansion. Its basis vectors $\{\phi_k\}$ are orthogonal in the Hilbert space of square integrable functions, $L_2[0,l_x]$, and its expansion coefficients $\xi_k(\omega)$ are also orthogonal (uncorrelated) in the Hilbert space of second-order random variables. It is this dual property that sets the KL-expansion apart from other orthogonal representations. Moreover, the KL-expansion is an optimal representation of $\Sigma(x,\omega)$ in the sense that it satisfies the following mean-square error minimizing property. If $\Sigma_K(x,\omega)$ is a generalized Fourier representation of the cross section to order K, then, for any other linear combination of functions, the error $||\Sigma - \Sigma_K||_2$ is larger than that obtained using the KL-expansion [3–5]. Thus, of all truncated spectral expansions of the cross section, the KL-expansion is the best in the mean-square sense.

The random expansion coefficients $\xi_k(\omega)$ are obtained by projecting Eq.(12) over $\phi_k(x)$ and using the orthogonality condition in Eq.(11) to get,

$$\xi_k(\omega) = \frac{1}{\sqrt{\lambda_k}} \int_0^{l_x} \tilde{\Sigma}(x,\omega)\,\phi_k(x)\,dx, \quad k = 1,2,\ldots \tag{15}$$

It is not possible in general to obtain the pdf's of the individual expansion coefficients in closed form but in the special case that Σ is a Gaussian stochastic process, the ξ_k are not just uncorrelated but are *independent*

Gaussian random variables. For Σ a non-Gaussian stochastic process, the ξ_k are not statistically independent although, as noted above, they are uncorrelated. However, it is possible to generate the pdf's numerically from Eq.(15). Alternatively, various order statistical moments of the ξ_k can be constructed from moments of the underlying cross section $\Sigma(x,\omega)$ using Eq.(15).

In order to demonstrate the value of a KL-representation of the random cross section in the numerical solution of the transport equation, we first examine the spectral decomposition of a specific and commonly used covariance function, an exponentially decaying function:

$$C_\Sigma(|x-x'|) = \langle\tilde{\Sigma}^2\rangle \exp\left(-\frac{|x-x'|}{\lambda_c}\right). \tag{16}$$

In Eq.(16), $\langle\tilde{\Sigma}^2\rangle$ is the variance and λ_c is a correlation length defined such that for $|x-x'| \gg \lambda_c$ cross section values at x and x' become independent. Thus, for $\lambda_c \to \infty$ the cross section is fully correlated over the entire slab, i.e., it shows no spatial structure, and reduces to a univariate random variable. On the other hand, for $\lambda_c \to 0$, the cross section at each spatial point is random but independent of its value at every other spatial location, and individual realizations have considerable spatial structure. These features will be reflected in the eigenstructure of the covariance operator in Eq.(10) which we numerically investigate next.

It is not difficult to show [3] that for an exponential covariance function the Fredholm integral equation Eq.(10) can be converted to a classical Sturm-Liouville boundary value problem. This can be achieved by unfolding the absolute value in the kernel in Eq.(10), differentiating twice with respect to x, and then rearranging to obtain:

$$\frac{d^2 f}{dx^2} + \alpha^2 f = 0, \qquad 0 \le x \le l_x, \tag{17}$$

with the homogeneous boundary conditions:

$$f'(0) - \frac{1}{\lambda_c} f(0) = 0, \tag{18}$$

$$f'(l_x) + \frac{1}{\lambda_c} f(l_x) = 0, \tag{19}$$

and where,

$$\alpha^2 = \frac{1}{\gamma\lambda_c}(2 - \frac{\gamma}{\lambda_c}), \qquad \gamma = \frac{\lambda}{\langle\tilde{\Sigma}^2\rangle}. \tag{20}$$

The eigenvalue λ corresponds to the values of α for which there exist nontrivial solutions to Eqs.(17) – (19) and these solutions are the unnormalized eigenfunctions. The eigenvalues must be numerically computed as the countably infinite roots of the following transcendental equation:

$$\tan(\alpha_n\, l_x) = \frac{2\,\alpha_n\lambda_c}{\alpha_n^2\lambda_c^2 - 1}, \qquad \lambda_n = \frac{2\,\langle\tilde{\Sigma}^2\rangle\lambda_c}{1 + \lambda_c^2\alpha_n^2}, \quad n = 1, 2, \ldots \tag{21}$$

The corresponding eigenfunctions are given by:

$$f_n(x) = \sin(\alpha_n x) + \alpha_n\lambda_c \cos(\alpha_n x), \quad n = 1, 2, \ldots \tag{22}$$

which can be normalized to yield the orthonormal eigenfunctions used in the KL-expansion, i.e.,

$$\phi_n(x) = \frac{f_n(x)}{||f_n||_2}, \quad n = 1, 2, \ldots \tag{23}$$

As an illustration, the first ten eigenvalues are plotted in Fig.(1) for a slab thickness $l_x = 10$cm, a cross section variance $\langle \tilde{\Sigma}^2 \rangle = 2\text{cm}^{-2}$, and a range of correlation lengths, $\lambda_c = 1 - 10$cm. We see that the eigenvalues decay monotonically with increasing n and that the lowest eigenvalue λ_1 becomes dominant for large λ_c values. The larger the λ_c, the steeper the decay of the eigenvalues. For small values of λ_c, on the other hand, all the eigenvalues are small and of comparable magnitude. It would be very useful for purposes of analysis to make explicit the asymptotic behavior of the eigenvalues for large and small λ_c.

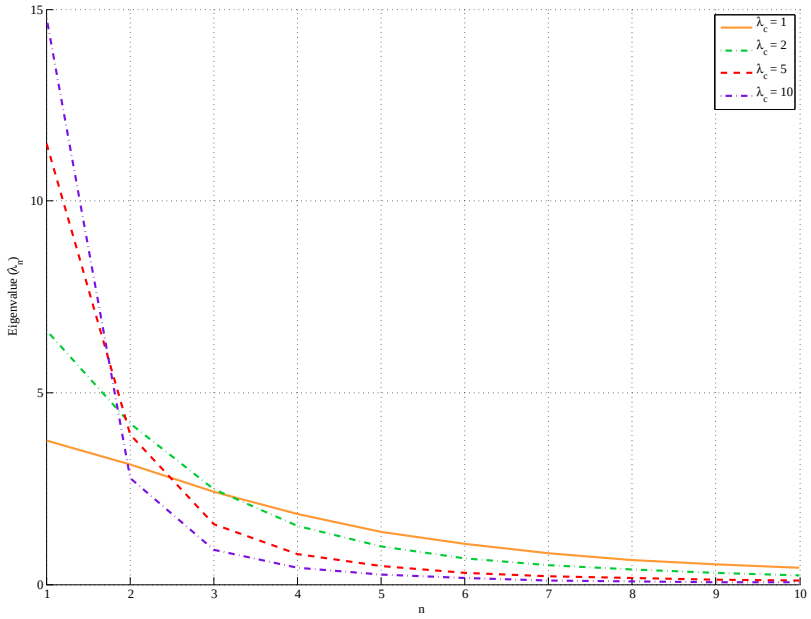

Figure 1. Eigenvalues ($l_x = 10$cm, $\langle \tilde{\Sigma}^2 \rangle = 2$cm)

The practical significance of this result is that it is possible to truncate the KL-expansion of the cross section and capture the dominant components of an infinite-dimensional process with surprisingly few modes, depending on the correlation length. In general, the more localized the covariance function C_Σ, i.e., the smaller the correlation length, the slower the decay of the eigenvalues and the more terms need to be retained in the KL-expansion. Thus the utility of this approach rests on the assumption that the cross section realizations vary smoothly, that is, there are significant correlations in the random field. Under such conditions, it is anticipated that a low order truncation can capture most of the uncertainty in the process. As we are dealing with physical systems, these conditions are presumed extant in our application. We demonstrate this for a cross section that is a Gaussian stochastic process with specified mean, variance and correlation length. In this case the expansion coefficients in the KL-expansion are independent, zero-mean Gaussian random variables with unit variance and a pdf given by:

$$P(\xi_k) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\xi_k^2}{2}\right), \quad -\infty < \xi_k < \infty, \quad k = 1, 2, \ldots. \tag{24}$$

Several realizations of the cross section computed from Eq.(12) are plotted in Fig.(2) for $\lambda_c = 2$cm for different KL-expansion orders and with $\langle \Sigma \rangle = 5\text{cm}^{-1}$ and $\langle \tilde{\Sigma}^2 \rangle = 2\text{cm}^{-2}$. The realizations display greater spatial structure with increasing number of terms in the expansion but are evidently all smooth.

To summarize, we have shown that the KL-decomposition provides an efficient dimension reducing

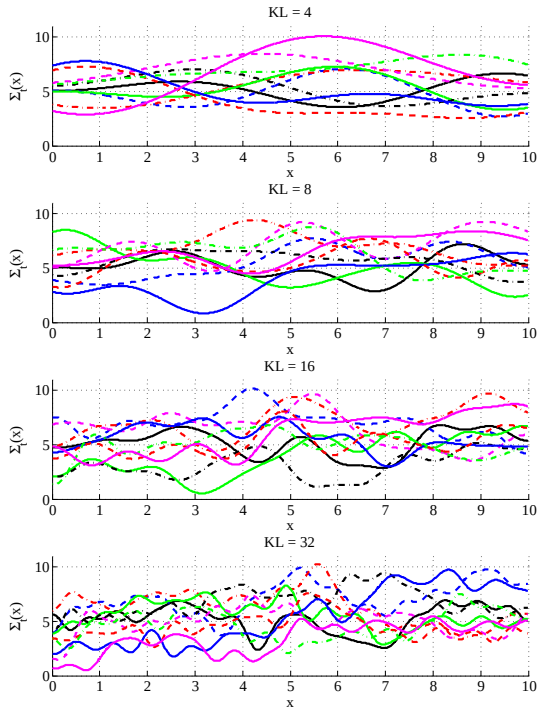

Figure 2. Cross Section Realizations: $\lambda_c = 2$ cm

representation of the spatially random cross section that has attractive properties for computation. We are now in a position to test its utility in the solution of our transport problem.

4. NUMERICAL SOLUTION OF RANDOM TRANSPORT EQUATION

Although representing Ψ in a KL-expansion may be feasible in principle (subject to the technical conditions described earlier), it is not a viable proposition for numerical implementation since its covariance function is not known a priori. Thus the value of the KL-expansion lies in simplifying the representation of otherwise numerically intractable random coefficients in the transport equation. Accordingly, the starting point of our numerical investigations is Eq.(1) with the total cross section given by the truncated KL-expansion,

$$\Sigma(x,\omega) = \langle\Sigma\rangle + \sum_{k=1}^{K} \sqrt{\lambda_k}\,\phi_k(x)\,\xi_k(\omega). \tag{25}$$

We assume the exponential covariance given in Eq.(16) so that the eigenvalues and eigenfunctions to be used in Eq.(25) are given by Eqs.(21) – (23). The random expansion coefficients $\xi_k(\omega)$ are defined by Eq.(15) and characterization of their statistical properties (moments, pdf's) is a crucial step in rendering the KL-representation practical for numerical work. As pointed out earlier, in general this can only be done by numerically evaluating Eq.(15) repeatedly for each mode. For the illustrative purposes of this article, however, we will consider the cross section fluctuations to be Gaussian distributed at every spatial location,

in which case the $\xi_k(\omega)$ are all zero-mean, unit variance i.i.d Gaussian random variables. Thus, realizations of the total cross section in Eq.(1) can be easily created by sampling a standard normal distribution $N(0,1)$ K times and evaluating the KL-expansion in Eq.(25). This approach will be used below for generating and analysing realizations of the scalar flux but, for computation of the mean scalar flux, use of quadratures proves to be computationally much more efficient than realization averaging in this case. The randomness in the angular flux can be functionally expressed as a parametric dependence on the K random variables $\{\xi_k(\omega)\}_1^K$, i.e., $\Psi(\omega) \equiv \Psi\left(\xi_1(\omega), \ldots \xi_K(\omega)\right)$. The expectation of any function of Ψ can then be written as:

$$\begin{aligned}\langle F(\Psi)\rangle &= \int\cdots\int F[\Psi(\xi_1,\ldots\xi_K)]P_K(\xi_1,\ldots\xi_K)\,d\xi_1\ldots d\xi_K \\ &= \int\cdots\int F[\Psi(\xi_1,\ldots\xi_K)]P(\xi_1)\ldots P(\xi_K)\,d\xi_1\ldots d\xi_K \end{aligned} \tag{26}$$

where in the second line above we have noted the independence of the random variables in factoring the multivariate pdf P_K into a product of K identical univariate pdf's each of which is $N(0,1)$, as given in Eq.(24) Thus the K-dimensional integral is actually K nested 1D integrals over the real line each with a Gaussian weight function. A natural quadrature rule for evaluating these integrals is Gauss-Hermite quadrature which, in the univariate case, returns an exact value with N quadrature points if the flux is a polynomial of degree $2N-1$ in the random variable. The numerical algorithm then reduces to solving a number of independent or uncoupled deterministic transport equations with the total cross section expressed as a truncated KL-expansion and the coefficients evaluated at Gauss-Hermite quadrature points. The mean flux is obtained by summing up these independent solutions weighted by the quadrature weights. As will be seen in the numerical results section, the number of times the transport equation must be solved to get good accuracy can be surprisingly small. Finally, the deterministic transport equation for each value of the cross section is solved using a discrete ordinates S_N discretization in angle and a linear discontinuous finite element representation in space with S_2-accelerated source iteration.

The convergence of the mean scalar flux to the true solution is guaranteed by the KL theorem with a sufficiently refined quadrature set, and the rate of convergence can be estimated with respect to standard norms, but in order to establish the accuracy of the solution for fixed expansion and quadrature order, it is necessary to compare against an exact solution. It has been shown by Prinja and Gonzalez-Aller [6] that, for Gaussian distributed density fluctuations and when the medium is source-free and of semi-infinite extent, an exact equation for the mean angular flux can be obtained. Unfortunately, the result is not a simple renormalized transport equation but rather has several complicating features that would require a nontrivial modification of the standard numerical algorithm. This is beyond the scope of this article, but, for the special case of a rod-model (also S_2) the result simplifies to the standard form and in this limit at least it is possible to compute the exact solution and use it as a benchmark. With $\langle\Psi^+\rangle$ denoting the mean flux in the forward direction and $\langle\Psi^-\rangle$ the flux in the backward direction, the closed equations for the rod model may be written as [6]:

$$\frac{\partial\langle\Psi^+\rangle}{\partial x} + \left[\langle\Sigma\rangle - (1-c)C_0(x)\right]\langle\Psi^+\rangle = \frac{c}{2}\langle\Sigma\rangle(\langle\Psi^+\rangle + \langle\Psi^-\rangle), \quad \langle\Psi^+\rangle(0) = 1, \tag{27}$$

$$-\frac{\partial\langle\Psi^-\rangle}{\partial x} + \left[\langle\Sigma\rangle + (1-c)C_0(x)\right]\langle\Psi^-\rangle = \frac{c}{2}\langle\Sigma\rangle(\langle\Psi^+\rangle + \langle\Psi^-\rangle), \quad \langle\Psi^-\rangle(l_x) = 0, \tag{28}$$

where C_0 is related to the covariance function through:

$$C_0(x) = \int_0^x C_\Sigma(x')dx', \tag{29}$$

and the mean scalar flux is given by:

$$\langle\Phi\rangle = \langle\Psi^+\rangle + \langle\Psi^-\rangle. \tag{30}$$

For computations, C_0 was obtained in closed form using the exponential covariance in Eq.(16) and numerically approximated as a piecewise constant function with the correct average value assigned to each spatial cell. Also, Eqs.(27) – (28) were discretized using the same linear discontinuous finite element scheme and solved by direct inversion to obtain all the cell unknowns simultaneously.

5. NUMERICAL RESULTS AND DISCUSSION

The mean scalar flux is shown in Fig.(3) as a function of depth into the medium for $\langle\Sigma\rangle = 5.0$cm, $c = 0.6$, $\lambda_c = 1.0$cm, $\langle\tilde{\Sigma}^2\rangle = 2\text{cm}^{-2}$, and various KL and quadrature orders. The results are compared against the exact result obtained from a numerical solution of Eqs.(27) – (28) for a semi-infinite medium. The deterministic solution ($\Sigma(x,\omega) = \langle\Sigma\rangle$) is also shown in order to provide a contrast with the nonrandom case. It is apparent that the numerical solution shows greater sensitivity to the quadrature order than to the KL order in the convergence to the exact solution. While a quadrature order of 6 is necessary to achieve an L_2 error of less than 1%, it appears that even two terms in the KL expansion are sufficient for capturing the effect of cross section uncertainty on the mean scalar flux. Furthermore, this conclusion is independent of the quadrature order. The deterministic solution is grossly in error away from the left slab face showing the inadequacy of a simple minded treatment of randomness. The apparent accuracy of the deterministic solution at and very near the left face is because of the fortuitous result that the surface scalar flux is nonrandom for a semi-infinite medium when only the density is a random function of position [2]. Although not shown for the mean scalar flux, for larger values of c, i.e., increased scattering, a quadrature and KL order of 2 generally proves sufficient. Overall it appears that dimension reduction followed by quadrature averaging is a fairly efficient approach when scattering is not insignificant.

Spatial scalar flux realizations for different cross section realizations, sampled from the truncated KL-representation, were computed as a function of the mean cross section, the variance and the correlation length. Very interesting results were obtained in particular when parameter choices were such that the corresponding deterministic case, with the total cross section given by the mean value, showed a diffusion limit. In the random case, the standard diffusion scalings:

$$\langle\Sigma\rangle \sim O\left(\frac{1}{\epsilon}\right), \quad (1-c) \sim O\left(\epsilon^2\right), \quad Q \sim O\left(\epsilon\right), \quad \epsilon \ll 1, \tag{31}$$

were introduced for each realization, but additionally the variance was also allowed to grow in proportion to the mean:

$$\langle\tilde{\Sigma}^2\rangle \sim O\left(\frac{1}{\epsilon}\right). \tag{32}$$

All other variables including the correlation length were assumed to be $O(1)$ quantities, i.e., $\lambda_c \gg \epsilon$ was assumed. Numerical results for several realizations are displayed in Figs.(4) and (5) for KL orders of 4 and 8, respectively. In both cases, $\lambda_c = 2$cm and the results in the top panel of each figure correspond to $\langle\Sigma\rangle = 5.0\text{cm}^{-1}$ and $\langle\tilde{\Sigma}^2\rangle = 2\text{cm}^{-2}$. The plots in the other panels in each figure show the same scalar flux realizations for decreasing values of ϵ in powers of two. These figures reveal the following very interesting observations, independent of the S_N order:

- The statistical noise in each scalar flux realization decreases with decreasing ϵ, to the point that the solutions appear to reach a "quiescent" state, i.e., a *nonrandom* solution is reached, regardless of the KL order.
- All realizations limit to the *same* nonrandom or deterministic flux shape.

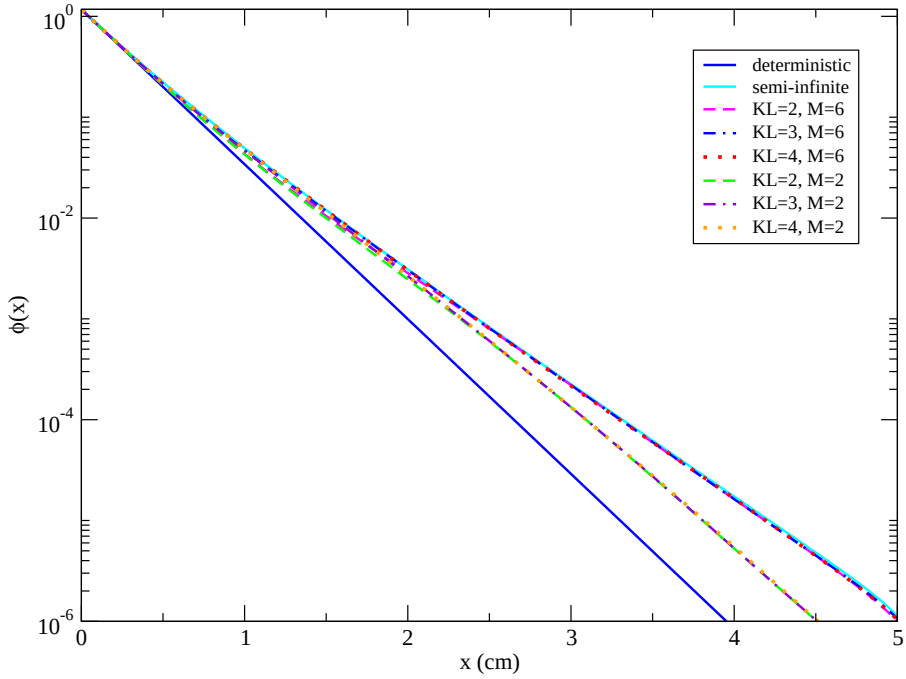

Figure 3. Mean Scalar Flux as a Function of KL and Quadrature Orders: c=0.5, $\lambda_c = 1$, cm

- This limiting flux shape is identical to that obtained from a diffusion equation with homogeneous flux boundary conditions and a diffusion coefficient given by $D = \frac{1}{3\langle\Sigma\rangle}$, i.e., to the scalar flux solution obtained for diffusion in a deterministic medium with a total cross section given by the mean cross section.

We emphasize that the above results were not obtained in the small noise limit but rather for very large fluctuations, as indicated by the scaling of the variance in Eq.(32). Also, a similar limit was observed for the mean angular flux, obtained by quadrature averaging: the mean angular flux asymptotically approached the mean scalar flux which in turn was equivalent to the scalar flux obtained from the deterministic diffusion equation. Significantly, this diffusion limit was also seen by Larsen [7, 8] earlier, for very different cross section statistics, namely alternating 1D layers of two different materials with exponentially distributed thicknesses. Larsen [7, 8] used asymptotic analysis to establish deterministic diffusion limits for both small and $O(1)$ correlation lengths. An asymptotic analysis of the model considered in this paper is currently underway in the hopes that a theoretical foundation for the observed numerical results can be established.

We further examined the L_2 norm of the difference between the scalar flux for each realization and the scalar flux obtained from the solution of the deterministic diffusion equation, i.e., $||\phi_K(x,\omega) - \phi_{diff}(x)||_2/||\phi_{diff}(x)||_2$, as a function of ϵ. The result for $K = 8$ is shown in Fig.(6) for

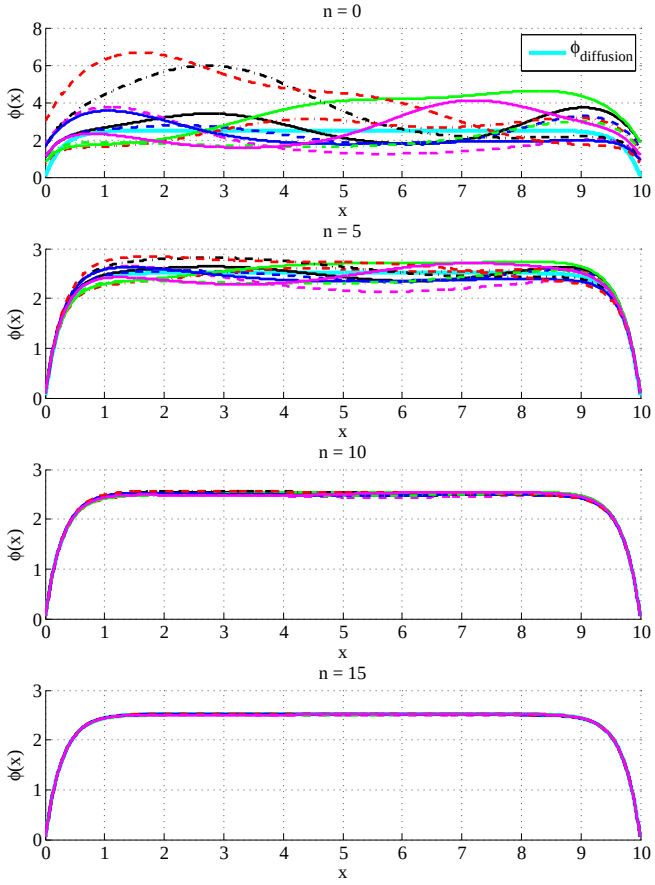

Figure 4. Scalar Flux Realizations: $\epsilon = 2^{-n}$, $\lambda_c = 2$cm, KL=4

twenty realizations. The difference norm for each realization decreases with ϵ, confirming our earlier conclusion that the scalar flux asymptotically approaches the diffusion scalar flux, but the figure also shows that $||\phi_K(x,\omega) - \phi_{diff}(x)||_2/||\phi_{diff}(x)||_2 \sim \sqrt{\epsilon}$ for every realization. This result is independent of the KL-expansion order and the S_N order. In contrast, the same difference norm when computed for the mean scalar flux shows $||\langle\phi_K(x)\rangle - \phi_{diff}(x)||_2/||\phi_{diff}(x)||_2 \sim \epsilon$, as shown in Fig.(7). Preliminary analysis shows that this difference can be traced to how the ϵ-scalings are manifested in the transport equation, with a strong clue provided by the exact ensemble averaged equations Eqs.(27) – (28). While the variance, which scales as $O(1/\epsilon)$, appears explicitly in these averaged equations, through $C_0(x)$ (see Eqs.(16) and (29)), it is the standard deviation that appears in the individual realizations, through the eigenvalues λ_k (see Eqs.(10),(16) and (21)), and this scales as $O(1/\sqrt{\epsilon})$. We strongly suspect that this difference in the scalings of the terms that describe the effects of randomness in the respective equations for individual realizations and the mean is responsible for the observed difference in the rates of convergence to the diffusion result. The aforementioned asymptotic analysis of the suitably scaled equations will also provide

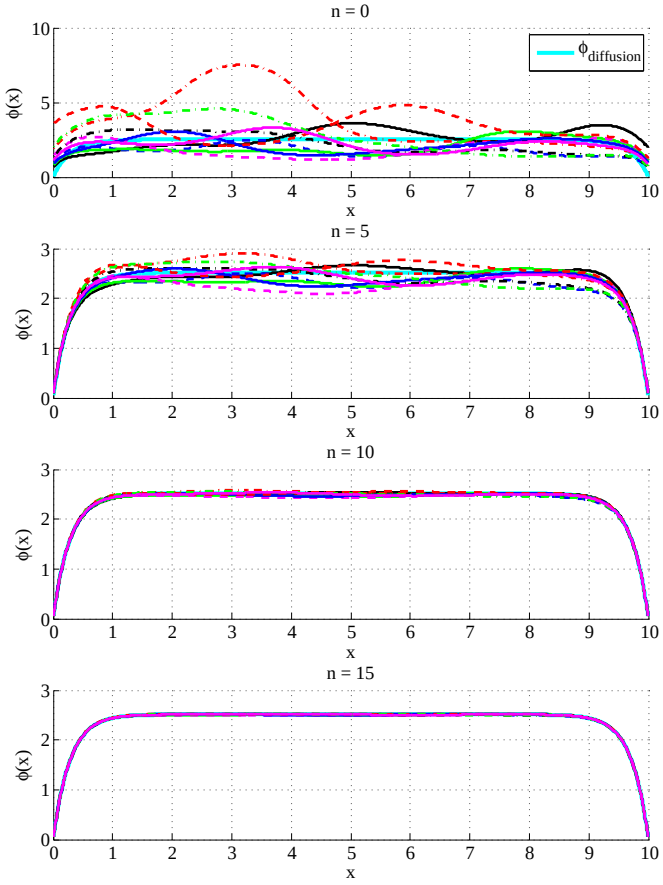

Figure 5. Scalar Flux Realizations: $\epsilon = 2^{-n}$**,** $\lambda_c = 2$**cm, KL=8**

a theoretical explanation for these numerical observations.

In concluding this paper, we make two final remarks. First, given that the limit to a nonrandom diffusion solution for a strongly fluctuating, scattering dominated, optically thick (with respect to the mean cross section) system, has been observed for two very different random cross section models, this result may in fact be a universal result. That is, the limit may be independent of the detailed distribution of cross section fluctuations and depend only on gross parameters such as the variance and the correlation length. It is not clear that this can be proved theoretically but obviously the cross section decomposition method demonstrated here can be applied to other types of random cross sections to address this possibility, in one as well as higher dimensions. Second, the so-called "atomic mix" limit corresponding to $\lambda_c = 0$ [2] cannot be demonstrated numerically using the KL-expansion method because of the increasing number of terms that need to be retained in the expansion with decreasing correlation length (see Fig.(1)). Even when the associated random coefficients are independent random variables, the number of transport equations

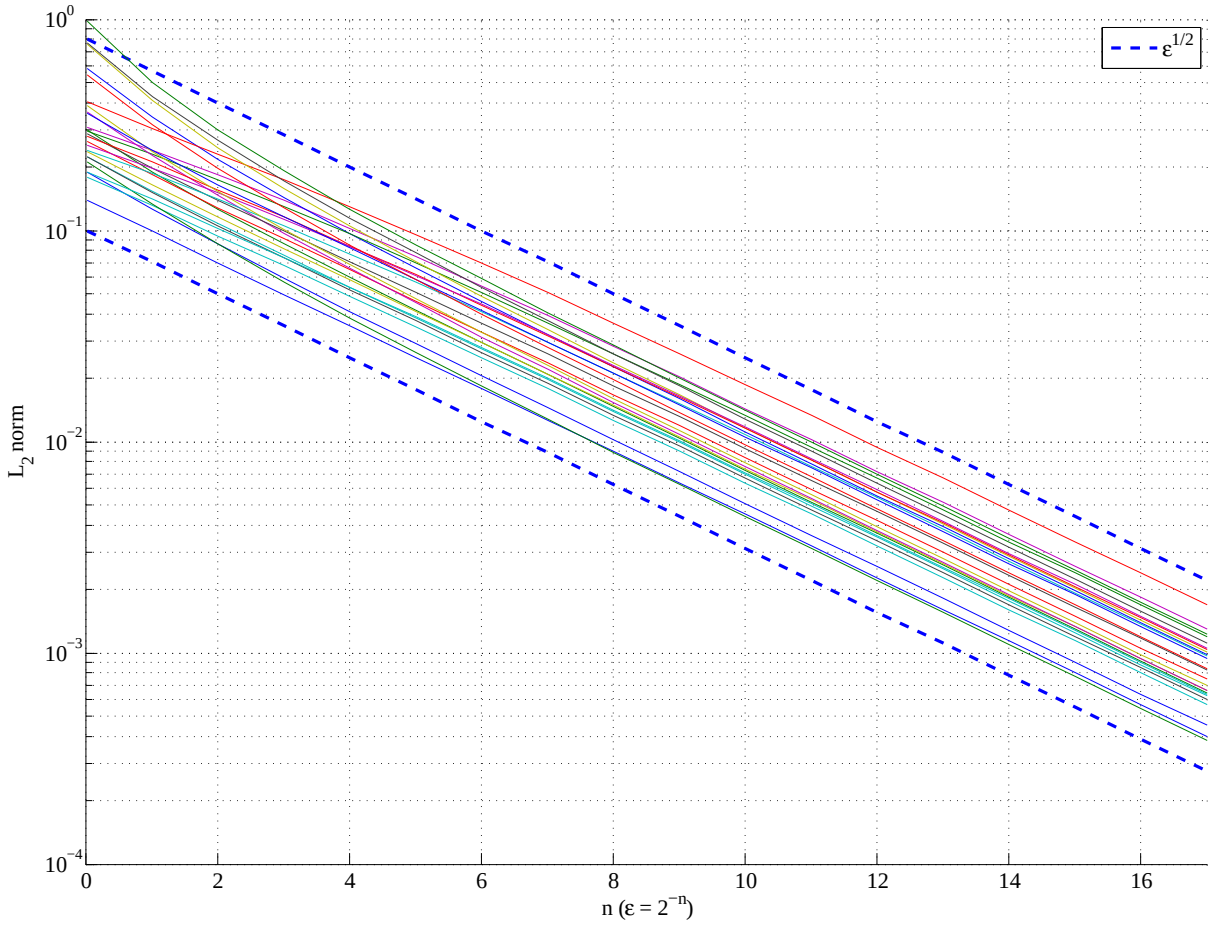

Figure 6. Scalar Flux Norm: $\epsilon = 2^{-n}$, $\lambda_c = 2$cm, KL=8

required to be solved will be intractably large. It should be possible, however, to prove this result theoretically, again using asymptotics, if the dependence of the KL eigenvalues can be made explicit in the small λ_c limit. This investigation is currently under way.

6. CONCLUSIONS

1. The Karhunen-Loève expansion provides an efficient eigenmode representation of random cross sections which are spatially continuous second order random processes. A relatively low order truncation of this expansion is possible when there exist non-negligible correlations in the physical property fluctuations.

2. With a low order KL-truncation, quadrature-based methods can provide an efficient alternative to realization averaging for numerical computation of the mean angular flux.

3. Surprisingly low order expansion and quadrature orders are needed for adequately capturing the

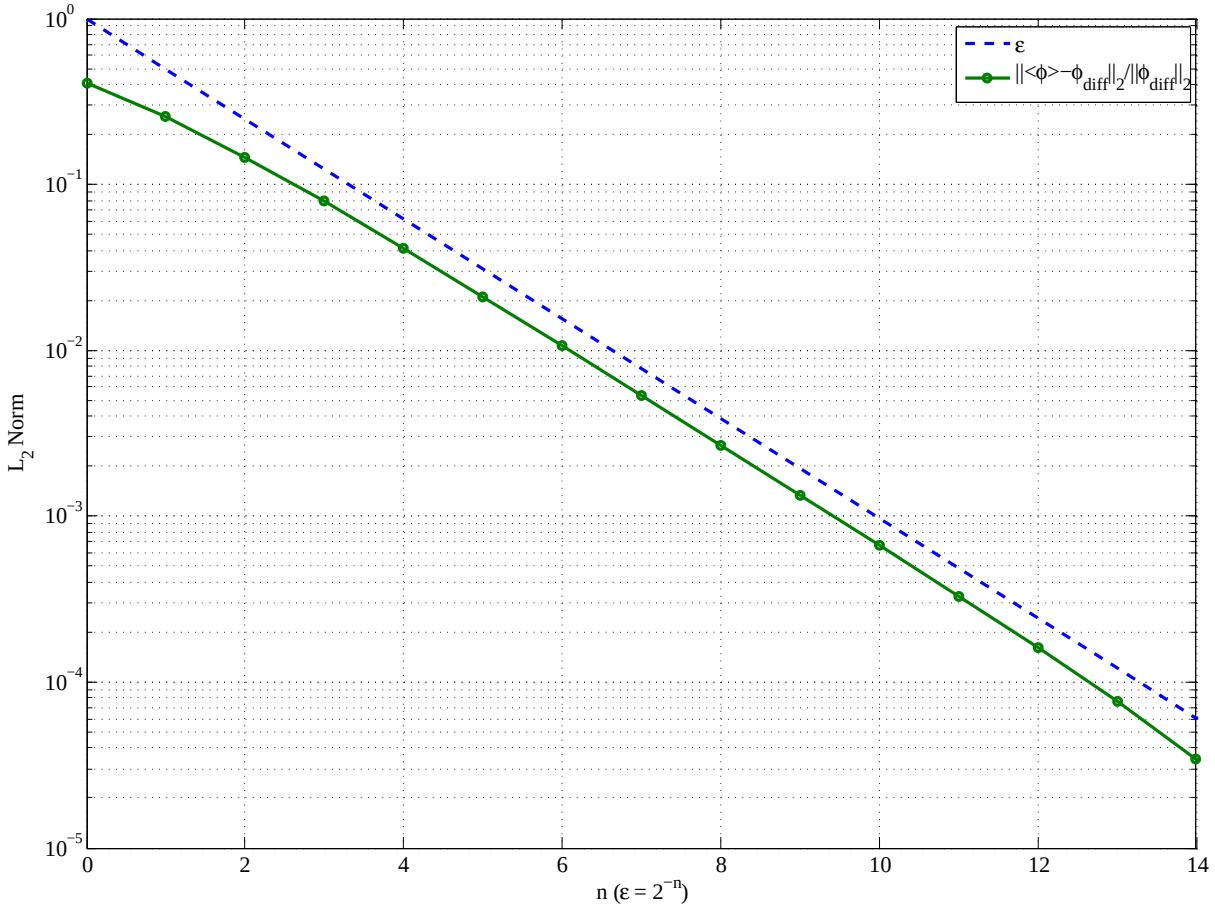

Figure 7. Mean Scalar Flux Norm: $\epsilon = 2^{-n}$**, c = 0.5,** $\lambda_c = 1$**cm**

effect of cross section uncertainty in the mean scalar flux, even when scattering does not dominate.

4. If the medium is a strong scatterer and is optically thick with respect to the mean cross section, the random transport equation is accurately approximated by a deterministic diffusion equation. This is true without restriction of the variance to a perturbative influence such that the original random problem is nearly deterministic. The asymptotic approach to a nonrandom diffusive solution was demonstrated for O(1) variance-to-mean ratio.

5. The realization specific scalar flux shows a much slower asymptotic approach to the nonrandom diffusion result than does the mean scalar flux.

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