The stochastic collocation method for radiation transport in random media

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ABSTRACT

Stochastic spectral expansions are used to represent random input parameters and the random unknown solution to describe radiation transport in random media. The total macroscopic cross section is taken to be a spatially continuous log-normal random process with known covariance function and expressed as a memoryless transformation of a Gaussian random process. The Karhunen–Loève expansion is applied to represent the spatially continuous random cross section in terms of a finite number of discrete Gaussian random variables. The angular flux is then expanded in terms of Hermite polynomials and, using a quadrature-based stochastic collocation method, the expansion coefficients are shown to satisfy uncoupled deterministic transport equations. Sparse grid Gauss quadrature rules are investigated to establish the efficacy of the polynomial chaos-collocation scheme. Numerical results for the mean and standard deviation of the scalar flux as well as probability density functions of the scalar flux and transmission function are obtained for a deterministic incident source, contrasting between absorbing and diffusive media.

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1. Introduction

The mathematical modeling of a broad range of physical phenomena requires the use of random differential, integral, or integro-differential operators. In radiation transport applications, randomness may reflect uncertainty in microscopic cross sections resulting from limited accuracy of experimental measurements or of underlying nuclear models. It may also result from material density fluctuations, for example turbulent mixing in atmospheric and stellar media, Rayleigh–Taylor unstable media [1,2], and random distribution of nuclear fuel in advanced fission reactor designs [3]. Work to date

on radiation transport in random media has heavily focused on binary statistical mixtures of immiscible materials. The binary mix model has been used for modeling cloudy atmospheres [4] and mixing zones at ICF fusion pellet interfaces [5]. In such applications, the randomness in the material density, and hence cross sections, arises from the random distribution of material interfaces, with the density being a deterministic quantity within each material. In this paper, on the other hand, we will consider the case in which material properties vary *continuously* as a function of space with a well-defined spatial correlation function. An alternative, more fundamental view of transport in random media, especially relevant in the characterization of clouds for atmospheric radiative transfer, can be found in [6].

Regardless of the source and type of parametric uncertainty, the solution, numerical or otherwise, of stochastically posed problems requires the physical parameters to be expressed as random variables, or

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random processes if the randomness has spatial and/or temporal dependence. Appropriate orders of moments, correlations and probability distribution functions of all input random parameters are assumed available and the level of detail of the statistics necessary to solve a particular problem will depend on the level of sophistication of the solution technique one is willing to employ. For instance, in direct sampling or Monte Carlo methods, the input parameters must be repeatedly sampled to generate a sufficiently large ensemble of solutions from which averages and probability distributions of output variables, as well as functionals of these variables, can be constructed. Thus, in this case, the input parameter uncertainty must be maximally characterized and expressed in the form of probability distribution functions. However, the cost of routinely applying such Monte Carlo methods can be prohibitively high. At the other extreme, closure methods, which seek to obtain a small number of approximate but deterministic equations directly for the mean and possibly also for the variance or correlation, rely only on low-order input parameter statistical information. This feature makes the approach computationally very attractive and suitable for developing insight into the effects of parametric stochasticity and, under specialized circumstances, generating analytical solutions. 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 Levermore–Pomraning closure [1], for instance, which was developed to describe radiation transport in random binary mixtures, is an exact closure when the material mixing is Markovian and all materials are purely absorbing. However, when either of these restrictions is violated, the closure can give highly inaccurate results [1] and has proved notoriously difficult to generalize.

A desirable methodology, then, is one capable of yielding accuracy potentially rivaling that of direct sampling methods but at a fraction of the computational cost, ideally, comparable to the cost of closure-based methods. In recent years, stochastic spectral methods [7–10] using the so-called polynomial chaos expansions (PCE) have been demonstrated to achieve high accuracy and computational efficiency, and have gained widespread popularity for solving physical problems formulated with random operators. The essence of this approach is the expansion of the random field representing the unknown solution in terms of random orthogonal basis functions and then reformulating the problem in terms of the unknown, but now deterministic, expansion coefficients. Equations for the latter can be obtained either by effecting Galerkin projections over the random basis functions, a technique that is known as the stochastic finite element method (SFEM) [7,8], or by applying a quadrature-based collocation method in the random dimension, a technique that is known as the stochastic collocation method (SCM) [11]. These techniques have met with considerable success in computational fluid dynamics and structural mechanics applications in particular, providing a robust methodology for uncertainty propagation and quantification, and there is now increasing interest in applying stochastic spectral methods to solve the stochastic radiation transport equation [9,10,12].

In this article, we apply the PCE-SCM method to the numerical solution of the linear transport equation when the atomic density of the medium is a continuous random function of position with log-normal probability distribution. That is to say, the atomic density and by extension the macroscopic cross section are random processes that are described at each point in the domain by a log-normal distribution. Since the underlying random process is Gaussian, the distribution is entirely characterized by its mean and covariance function. The covariance function describes how rapidly two points on the spatial domain become statistically independent and in most physical applications this effect is conveniently captured by a correlation length (we describe this in detail below for a specific application). Key to the numerical solution of randomly posed problems of the type considered in this paper is the ability to efficiently and accurately represent continuous random processes. Although it is possible in principle to construct realizations of correlated Gaussian processes directly on a grid (as demonstrated below), in practice this procedure can be computationally inefficient and it is desirable to first use a so-called dimension reducing technique such as the Karhunen–Loève (KL) transform [13]. We defer a detailed discussion of this method to an appropriate point in the paper, but we note here that the KL transform accurately approximates a continuous Gaussian random process by a finite linear combination of independent Gaussian random variables, thereby making it particularly straightforward and efficient to generate numerical realizations of Gaussian processes, as well as nonlinear functions and functionals of such processes.

The advantage of the log-normal process over the Gaussian is that its support is non-negative so that, unlike with the Gaussian distribution, negative cross section values cannot occur. Thus, large atomic density variances can be accommodated without incurring the complication of unphysical artifacts commonly associated with Gaussian representations of highly variable physical data [14]. This enables a systematic investigation to be conducted of the effect of parametric uncertainty on the statistics of the output variables and on the numerical efficiency of the spectral representation. The KL representation is easily obtained by first generating the expansion for the associated Gaussian random process and then applying a suitable nonlinear transformation. Once the KL expansion is generated, collocations of the random variables can be constructed using multidimensional Gauss quadrature rules for use in the PCE-SCM approach. As will be shown, however, the product quadrature sets expand rapidly with increasing numbers of random variables in the KL representation of the original random process and it becomes essential to employ a sparse grid quadrature method for the SCM approach to remain computationally viable.

The scope of the paper is as follows. The stochastic transport problem is defined and discussed in Section 2 followed by a presentation of the Karhunen–Loève