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VARIANCE ESTIMATES FOR TRANSPORT IN STOCHASTIC MEDIA BY MEANS OF THE MASTER EQUATION

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ABSTRACT

The master equation has been used to examine properties of transport in stochastic media. It has been shown previously that not only may the Levermore-Pomraning (LP) model be derived from the master equation for a description of ensemble-averaged transport quantities, but also that equations describing higher-order moments may be obtained. We examine in greater detail the equations governing the second moments of the angular fluxes, from which variances may be computed. We introduce a simple closure for these equations, as well as several models for estimating the variances of derived transport quantities. We revisit previous benchmarks for transport in stochastic media in order to examine the error of these new variance models. We find, not surprisingly, that the errors in these variance estimates are at least as large as the corresponding estimates of the average, and sometimes much larger. We also identify patterns in these variance estimates that may help guide the construction of more accurate models.

Key Words: radiation transport, stochastic media, benchmarks, master equation

1. INTRODUCTION

Various transport problems of practical interest involve background media consisting of a mixture of two or more well-characterized materials whose spatial distribution is known only in a statistical sense. Examples of such problems include the transport of solar radiation through cloudy atmosphere and the neutron distribution in pebble bed reactors. Given knowledge of the statistical distribution of the materials in relevant physical realizations, the problem of transport through such stochastic media consists of determining the statistical distribution of angular fluxes and derived quantities such as dose in these realizations. For example, one may wish to determine the mean, variance, and maximum reactivity of a pebble bed reactor in order to ensure criticality safety during operation regardless of the physical arrangement of the pebbles.

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In principle one could generate physical realizations from a statistical description of the stochastic media, perform transport calculations on each realization, and then examine the ensemble results. Such an approach suffers from two problems. First, all but the simplest of realizations may be too complex to directly model. Second, the number of realizations required for good statistics may be computationally prohibitive. Therefore it is desirable to construct other methods that can yield the same information at less cost.

One such method that has been applied with varying success is the Levermore-Pomraning (LP) approach, sometimes referred to as the "standard model" [1-2]. This approach uses a single realization with material properties derived from the physical materials involved as well as the statistical distribution of the materials. In the special case of Markovian media with no scattering the LP model is exact. In addition to shortcomings related to inexact treatment of material boundaries, the LP model yields only ensemble-averaged quantities; higher statistical measures are not addressed.

A more comprehensive approach to the problem of transport through stochastic media makes use of a master equation. It has been shown that not only may the LP model be derived by means of this approach, but also equations describing higher-order quantities can be obtained [3]. The purpose of this paper is to examine this approach more closely, in particular in order to obtain variance estimates of transport quantities.

The rest of the paper is organized as follows. In Section 2 we first give an overview of previous work that forms the basis of our current work, then we present models for estimating the variance of transport results. In Section 3 we report numerical results using these new models along with analysis of their errors. In Section 4 we present conclusions and suggestions for future work.

2. THEORY

In this section we first review some previous analysis of the master equation approach to transport in stochastic media. We then introduce a simple closure for the equation governing the second-order moment of the angular fluxes, from which one can compute variances. We also introduce several models for estimating the variances of some derived transport quantities.

2.1. Previous Work

In Ref. [3] the master equation describing transport in stochastic media was derived from first principles, including the effects of scattering. One intermediate result, prior to the introduction of any approximations or closures, is

$$\begin{aligned} &\frac{1}{v}\frac{\partial}{\partial t}(p_i P_i) + \vec{\Omega}\cdot\nabla(p_i P_i) - \frac{\partial}{\partial \psi}[(\sigma_{ti}\psi - Q_i)p_i P_i] \\ &= \frac{p_j \bar{P}_j}{\lambda_j} - \frac{p_i \bar{P}_i}{\lambda_i} - \frac{\partial}{\partial \psi}\int_0^\infty dE' \int_{4\pi} d\vec{\Omega}' \int_0^\infty d\psi' \psi' \sigma_{si}\big(\vec{r}, E' \to E, \vec{\Omega}\cdot\vec{\Omega}'\big) p_i P_{2i}(\psi, \psi') \end{aligned} \quad (1)$$

where $p_i = p_i(\vec{r}), i = 1,2,...,$ is the probability that the point $\vec{r}$ lies in material i, $P_i = P_i(\psi)$ is the conditional probability density for the angular flux given that the point $\vec{r}$ lies in material i, $\bar{P}_i = \bar{P}_i(\psi)$ is the conditional probability density for the angular flux given that the point $\vec{r}$ lies on an interface exiting a region of material i, $P_{2i}(\psi,\psi')$ is the conditional joint probability density for the angular flux given that the point $\vec{r}$ lies in material i, and λ_i is the mean chord length for material i. Equation (1) exactly describes transport in stochastic media, but the terms $\bar{P}_i$ and P_{2i} render it stochastically unclosed.

In order to close Equation (1) we introduce the LP-closure of the material interface terms:

$$\frac{p_j\bar{P}_j}{\lambda_j} - \frac{p_i\bar{P}_i}{\lambda_i} \approx \frac{p_jP_j}{\lambda_j} - \frac{p_iP_i}{\lambda_i} \tag{2}$$

The approximation made in Equation 2 is that the statistical distribution of angular fluxes at material interfaces is identical to that of fluxes in the interior of material regions. Substitution of Equation (2) into Equation (1) yields the LP-closed master equation:

$$\begin{aligned}\frac{1}{v}\frac{\partial}{\partial t}(p_iP_i) + \vec{\Omega}\cdot\nabla(p_iP_i) - \frac{\partial}{\partial\psi}[(\sigma_{ti}\psi - Q_i)p_iP_i]\\ = \frac{p_jP_j}{\lambda_j} - \frac{p_iP_i}{\lambda_i} - \frac{\partial}{\partial\psi}\int_0^\infty dE'\int_{4\pi} d\vec{\Omega}'\int_0^\infty d\psi'\psi'\sigma_{si}\big(\vec{r},E'\to E,\vec{\Omega}\cdot\vec{\Omega}'\big)p_iP_{2i}(\psi,\psi')\end{aligned} \tag{3}$$

We define the conditionally averaged angular flux moments of order n:

$$\psi_i^{(n)} = \int_0^\infty d\psi\psi^nP_i \tag{4}$$

The first angular flux moment of Equation (3) is

$$\begin{aligned}\frac{1}{v}\frac{\partial}{\partial t}(p_i\psi_i) + \vec{\Omega}\cdot\nabla(p_i\psi_i) + \sigma_{ti}p_i\psi_i\\ = \frac{p_j\psi_j}{\lambda_j} - \frac{p_i\psi_i}{\lambda_i} + p_iQ_i + \int_0^\infty dE'\int_{4\pi} d\vec{\Omega}'\sigma_{si}\big(\vec{r},E'\to E,\vec{\Omega}\cdot\vec{\Omega}'\big)p_i\,\psi_i\end{aligned} \tag{5}$$

where $\psi_i \equiv \psi_i^{(1)}$. This is the familiar LP or "standard" model for ensemble-averaged angular fluxes. Note that the P_{2i} from Equation (3) are not present in Equation (5), so no further closures are necessary to determine ensemble-averaged fluxes.

Higher moments of Equation (3) are given by

$$\frac{1}{v}\frac{\partial}{\partial t}\left(p_i\psi_i^{(n)}\right) + \vec{\Omega}\cdot\nabla\left(p_i\psi_i^{(n)}\right) + n\sigma_{ti}p_i\psi_i^{(n)} = \frac{p_j\psi_j^{(n)}}{\lambda_j} - \frac{p_i\psi_i^{(n)}}{\lambda_i} + np_iQ_i\psi_i^{(n-1)} + n\int_0^\infty dE'\int_{4\pi} d\vec{\Omega}'\int_0^\infty d\psi\int_0^\infty d\psi'\psi^{n-1}\psi'\sigma_{si}\left(\vec{r},E'\to E,\vec{\Omega}\cdot\vec{\Omega}'\right)p_iP_{2i}(\psi,\psi') \tag{6}$$

Unlike Equation (5) the higher moment equations still include P_{2i} and thus require an additional closure. This is the subject of the next subsection.

2.2. Variance Models

2.2.1. Variance of angular fluxes

We propose the following partial correlation neglect model as a closure for Eq. (6):

$$P_{2i}(\psi,\psi') = \begin{cases} P_i(\psi')\delta(\psi-\psi'), & E'=E, \vec{\Omega}'=\vec{\Omega} \\ P_i(\psi)P_i(\psi'), & otherwise \end{cases} \tag{7}$$

In other words, the value of the flux in a given direction and of a given energy is perfectly correlated with itself, but is uncorrelated with fluxes at other energies or directions. Substitution of Equation (7) into Equation (6) for $n = 2$ yields

$$\begin{aligned}\frac{1}{v}\frac{\partial}{\partial t}\left(p_i\psi_i^{(2)}\right) &+ \vec{\Omega}\cdot\nabla\left(p_i\psi_i^{(2)}\right) + 2\sigma_{ti}p_i\psi_i^{(2)} \\ = \frac{p_j\psi_j^{(2)}}{\lambda_j} - \frac{p_i\psi_i^{(2)}}{\lambda_i} &+ 2p_iQ_i\psi_i + 2\int_0^\infty dE'\int_{4\pi} d\vec{\Omega}'\int_0^\infty d\psi\int_0^\infty d\psi'\psi\psi'\sigma_{si}\left(\vec{r},E'\to E,\vec{\Omega}\cdot\vec{\Omega}'\right)p_iP_i(\psi)P_i(\psi') \\ &- 2\int_0^\infty dE'\int_{4\pi} d\vec{\Omega}'\int_0^\infty d\psi\int_0^\infty d\psi'\psi\psi'\sigma_{si}\left(\vec{r},E'\to E,\vec{\Omega}\cdot\vec{\Omega}'\right)p_i\delta(E'-E)\delta\left(\vec{\Omega}'-\vec{\Omega}\right)P_i(\psi)P_i(\psi') \\ &+ 2\int_0^\infty dE'\int_{4\pi} d\vec{\Omega}'\int_0^\infty d\psi\int_0^\infty d\psi'\psi\psi'\sigma_{si}\left(\vec{r},E'\to E,\vec{\Omega}\cdot\vec{\Omega}'\right)p_i\delta(E'-E)\delta\left(\vec{\Omega}'-\vec{\Omega}\right)P_i(\psi')\delta(\psi-\psi')\end{aligned} \tag{8}$$

Simplification leads to

$$\begin{aligned}\frac{1}{v}\frac{\partial}{\partial t}\left(p_i\psi_i^{(2)}\right) &+ \vec{\Omega}\cdot\nabla\left(p_i\psi_i^{(2)}\right) + 2\sigma_{ti}p_i\psi_i^{(2)} \\ &= \frac{p_j\psi_j^{(2)}}{\lambda_j} - \frac{p_i\psi_i^{(2)}}{\lambda_i} + 2p_iQ_i\psi_i \\ &+ 2p_i\psi_i\int_0^\infty dE'\int_{4\pi} d\vec{\Omega}'\int_0^\infty d\psi'\psi'\sigma_{si}\left(\vec{r},E'\to E,\vec{\Omega}\cdot\vec{\Omega}'\right)P_i(\psi') \\ &- 2p_i\sigma_{si}(\vec{r},E\to E,1)\psi_i^2 + 2p_i\sigma_{si}(\vec{r},E\to E,1)\psi_i^{(2)}\end{aligned} \tag{9}$$

We restrict our attention to monoenergetic transport with isotropic scattering. After simplification Equation (9) becomes

$$\frac{1}{v}\frac{\partial}{\partial t}\left(p_i\psi_i^{(2)}\right)+\vec{\Omega}\cdot\nabla\left(p_i\psi_i^{(2)}\right)+2\sigma_{ai}p_i\psi_i^{(2)} \\ =\frac{p_j\psi_j^{(2)}}{\lambda_j}-\frac{p_i\psi_i^{(2)}}{\lambda_i}+2p_iQ_i\psi_i+2p_i\sigma_{s0,i}\psi_i(\varphi_i-\psi_i) \tag{10}$$

The variance of any particular angular flux may then be calculated in the usual manner:

$$\Sigma^2(\psi_i)=\psi_i^{(2)}-\psi_i^2 \tag{11}$$

2.2.2 Variance of derived quantities

In practical applications we are rarely interested in the statistics of individual angular fluxes. Rather we are often concerned with derived quantities such as dose or leakage. Mean quantities may be calculated in the same manner as for non-stochastic transport. Variance estimates, however, will require that we create models for combining the individual variances given by Equation (11), since we do not know how these individual variances are correlated. We restrict our attention to creating variance models for the quantities of interest reported in Ref. [4], namely reflection and transmission of monoenergetic particles in one-dimensional slab geometry. These quantities are computed from fluxes in different materials and directions, but at a single spatial location and energy. For example, reflection of particles incident from the left of the region of interest is given by

$$R=p_0R_0+p_1R_1=p_0\sum_{\mu_k>0}w_k\mu_k\psi_{k,0}(x_L)+p_1\sum_{\mu_k>0}w_k\mu_k\psi_{k,1}(x_L) \tag{12}$$

where w_k are the weights and μ_k the direction cosines of an angular quadrature. A similar equation holds for transmission.

We propose the following models for the variance of leakage from a surface in one-dimensional slab geometry, where the flux variances are evaluated at the relevant boundary:

zero correlation

$$\Sigma^2(L)=\sum_{\vec{\Omega_k}\cdot\vec{n}>0}w_k^2\,\mu_k^2\left(p_0^2\Sigma^2\left(\psi_{k,0}\right)+p_1^2\Sigma^2\left(\psi_{k,1}\right)\right) \tag{13a}$$

full correlation

$$\Sigma^2(L)=\left[\sum_{\vec{\Omega_k}\cdot\vec{n}>0}w_k\mu_k\left(p_0\Sigma\left(\psi_{k,0}\right)+p_1\Sigma\left(\psi_{k,1}\right)\right)\right]^2 \tag{13b}$$

average correlation

$$\Sigma^2(L)=\sum_{\vec{\Omega_k}\cdot\vec{n}>0}w_k\mu_k\left(p_0\Sigma^2\left(\psi_{k,0}\right)+p_1\Sigma^2\left(\psi_{k,1}\right)\right) \tag{13c}$$

hybrid correlation
$$\Sigma^2(L) = \sum_{\overrightarrow{\Omega_k}\cdot\vec{n}>0} w_k\mu_k\left(p_0^3\Sigma^2(\psi_{k,0}) + p_1^3\Sigma^2(\psi_{k,1})\right) \tag{13d}$$

3. NUMERICAL RESULTS

In order to test our new variance models we reexamine the stochastic media transport problems first reported in [4]. These problems consist of nine different combinations of binary media and mixing statistics. The problems are monoenergetic in one-dimensional slab geometry. Two different angular quadratures are used; the "rod" problems are equivalent to using a two-point Gauss-Lobatto quadrature, and the "planar" problems use an S_{16} Gauss-Legendre quadrature. The problems are driven by an isotropic flux on the left boundary, scaled so that the incident current is unity. All scattering is isotropic. The reflected and transmitted currents are the transport quantities examined.

Although both the ensemble-averages and deviations from benchmark calculations were reported in [4], we have separately regenerated the results as reported in [5]; the two sets of benchmarks are consistent with each other. We generate our results with the Sceptre deterministic code [6] using its discretization of the first-order form of the linear monoenergetic Boltzmann equation, controlling for iterative, spatial, and statistical error.

Both the LP model and our variance models were also implemented as separate modules of the Sceptre code base. Results from these models were generated for all of the test cases and their errors were computed by comparison with our benchmark results, which were solved to within 1% statistical error.

In this article we do not report the individual results for each stochastic problem. Rather we have generated condensed results by applying various metrics to the results of all nine cases simultaneously. To do this we first take the ratio of each transport quantity computed by our stochastic models and the benchmark results; a ratio of unity implies exact agreement of our models with the benchmark results. We then apply each of the following metrics to these ratios:

min:
$$\min(ratio_i)\,, i = 1..9 \tag{14a}$$

max:
$$\max(ratio_i)\,, i = 1..9 \tag{14b}$$

average:
$$exp\left[\frac{1}{9}\sum_{i=1}^{9}\ln(ratio_i)\right] \tag{14c}$$

norm:
$$exp\left[\frac{1}{9}\sum_{i=1}^{9}|\ln(ratio_i)|\right] \tag{14d}$$

Our results are reported for various slab thicknesses in Tables I-II for the rod problems and Tables III-IV for the planar problems. These results consist of both the LP-averages (previously reported) and the deviations as calculated by the models of Section 2.2.

Table I. Condensed statistical results for reflection, rod problem

Δx	metric	$\langle R \rangle$	$\Sigma(R)$-zero	$\Sigma(R)$-full	$\Sigma(R)$-average	$\Sigma(R)$-hybrid
0.1	min	0.985	0.112	0.159	0.159	0.079
	max	1.014	0.526	0.647	0.694	0.484
	average	0.995	0.220	0.285	0.301	0.185
	norm	1.009	4.540	3.511	3.327	5.407
1	min	0.893	0.275	0.383	0.389	0.194
	max	0.996	0.999	1.124	1.128	0.940
	average	0.938	0.492	0.606	0.616	0.419
	norm	1.066	2.034	1.738	1.712	2.389
10	min	0.670	0.272	0.355	0.385	0.193
	max	0.902	9.085	10.115	10.115	8.569
	average	0.774	0.838	1.005	1.021	0.716
	norm	1.291	2.170	2.037	2.006	2.472

Table II. Condensed statistical results for transmission, rod problem

Δx	metric	$\langle T \rangle$	$\Sigma(T)$-zero	$\Sigma(T)$-full	$\Sigma(T)$-average	$\Sigma(T)$-hybrid
0.1	min	0.999	0.108	0.152	0.152	0.076
	max	1.003	0.555	0.662	0.695	0.515
	average	1.001	0.223	0.286	0.300	0.188
	norm	1.001	4.489	3.492	3.336	5.330
1	min	0.997	0.342	0.473	0.484	0.242
	max	1.027	1.009	1.140	1.143	0.949
	average	1.008	0.581	0.708	0.719	0.496
	norm	1.009	1.724	1.488	1.466	2.017
10	min	0.955	0.711	0.860	1.006	0.503
	max	1.455	3.549	3.924	3.924	3.349
	average	1.168	1.310	1.522	1.560	1.124
	norm	1.190	1.446	1.574	1.560	1.562

Table III. Condensed statistical results for reflection, planar problem

Δx	metric	$\langle R \rangle$	$\Sigma(R)$-zero	$\Sigma(R)$-full	$\Sigma(R)$-average	$\Sigma(R)$-hybrid
0.1	min	0.965	0.041	0.150	0.250	0.125
	max	1.015	0.201	0.647	1.023	0.829
	average	0.986	0.082	0.274	0.456	0.291
	norm	1.018	12.198	3.646	2.213	3.442
1	min	0.839	0.096	0.337	0.557	0.315
	max	0.987	0.377	1.116	1.593	1.306
	average	0.910	0.178	0.564	0.882	0.603
	norm	1.099	5.610	1.851	1.424	1.861
10	min	0.655	0.099	0.323	0.625	0.312
	max	0.881	9.820	27.786	39.684	33.285
	average	0.751	0.353	1.092	1.679	1.179
	norm	1.332	4.709	2.217	2.038	2.116

Table IV. Condensed statistical results for transmission, planar problem

Δx	metric	$\langle T \rangle$	$\Sigma(T)$-zero	$\Sigma(T)$-full	$\Sigma(T)$-average	$\Sigma(T)$-hybrid
0.1	min	1.001	0.039	0.160	0.248	0.124
	max	1.004	0.220	0.672	1.021	0.789
	average	1.002	0.086	0.293	0.453	0.288
	norm	1.002	11.577	3.418	2.227	3.474
1	min	0.996	0.133	0.473	0.688	0.344
	max	1.051	0.406	1.159	1.656	1.373
	average	1.015	0.232	0.720	1.042	0.723
	norm	1.016	4.305	1.481	1.329	1.679
10	min	0.927	0.288	0.870	1.485	0.742
	max	1.767	2.530	6.497	10.265	8.755
	average	1.195	0.643	1.827	2.782	2.009
	norm	1.240	2.169	1.885	2.782	2.179

There are several conclusions we draw from these results. First, the errors in the deviations/variances are generally at least as large as the errors in the mean. This is not surprising, since the mean fluxes are used in the calculation of the variances. A related observation is that the models for both the mean and the variances tend to underestimate the results for thin problems and overestimate for thick problems; the results for the mean are driving the results for the variances. Secondly, the relative errors in the deviation are at times much larger than the corresponding errors in the mean. This also is not surprising, since the calculation of the variances involves two more closures or approximations than the calculation of the mean. Finally, the average correlation model for the variance (Equation (13c)) typically is the most accurate for reflection regardless of problem thickness, whereas for transmission the best variance model seems to transition from the average correlation model to the full correlation model (Equation (13b)) to the zero correlation model (Equation (13a)) as the problem size increases.

4. CONCLUSIONS

We have extended previous work on transport in stochastic media by proposing a closure model for the equation governing the second moment of the angular fluxes, as derived from a master equation for such problems. We furthermore have proposed several models for determining the variances of some particular integral transport quantities. The accuracy of these models has been evaluated against numerous benchmark problems. To our knowledge this is the first work to obtain higher-order results associated with the LP model for transport in stochastic media. The errors in the variances we have computed are generally worse than those for the mean; whether such errors are acceptable or not will depend on the nature of the problem and the desired accuracy.

There are several opportunities for improvements and future work. The first is improving the LP closure of Equation (2); improved models should increase the accuracy of both the mean and the variances. The second area of work is to obtain improved closures for the second-moment equation, particularly for energy-dependent problems and anisotropic scattering, which we have not examined. Finally, the variance estimates of Equations (13) are applicable only for certain transport quantities. New models for variances will need to be created for transport results that involve integrals over space and/or energy.

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REFERENCES

1. G.C. Pomraning, *Linear Kinetic Theory and Particle Transport in Stochastic Mixtures*, World Scientific, Singapore (1991).
2. R. Sanchez, "Linear Kinetic Theory in Stochastic Media," *J. Math. Physics*, **30**, pp. 2948-2511 (1989).
3. A.K. Prinja, "On the Master Equation Approach to Transport in Discrete Random Media in the Presence of Scattering," *Annals of Nuclear Energy*, **31**, pp. 2005-2016 (2004).
4. M.L. Adams, E. W. Larsen and G.C. Pomraning, "Benchmark Results for Particle Transport in a Binary Markov Statistical Medium," *J. Quant. Spectrosc. Radiat. Transfer*, **42**, pp. 253-266 (1989).
5. S.D. Pautz and B.C. Franke, "Generation of Accurate Benchmarks for Transport in Stochastic Media by Means of Dynamic Error Control," *Proc. Int. Conf. on Mathematics and Computational Methods Applied to Nuclear Science and Engineering*, Rio de Janeiro, Brazil (2011).

6. S. Pautz, B. Bohnhoff, C. Drumm and W. Fan, "Parallel Discrete Ordinates Methods in the SCEPTRE Project," *Proc. Int. Conf. on Mathematics, Computational Methods and Reactor Physics*, Saratoga Springs, NY, May 3-7, 2009.