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AN IMPROVED DETERMINISTIC METHOD FOR THE SOLUTION OF STOCHASTIC MEDIA TRANSPORT PROBLEMS

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ABSTRACT

We present an improved deterministic method for analyzing transport problems in random media. In the original method realizations were generated by means of a product quadrature rule; transport calculations were performed on each realization and the results combined to produce ensemble averages. In the present work we recognize that many of these realizations yield identical transport problems. We describe a method to generate only unique transport problems with the proper weighting to produce identical ensemble-averaged results at reduced computational cost. We also describe a method to ignore relatively unimportant realizations in order to obtain nearly identical results with further reduction in costs. Our results demonstrate that these changes allow for the analysis of problems of greater complexity than was practical for the original algorithm.

Key Words: radiation transport, stochastic media

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.

In previous work [1] we demonstrated that one can approximately calculate ensemble-averaged transport quantities for stochastic media problems by means of deterministically-generated realizations (as opposed to Monte Carlo sampling of realizations). Such realizations are characterized by the number and location of "pseudointerfaces" they contain and by the material assignments between pseudointerfaces. Appropriate weighting of such realizations yields an ensemble average whose accuracy is governed by the maximum number of pseudointerfaces, the quadrature order for spatial distribution of the pseudointerfaces, and the underlying material statistics. The expense of this method grows rapidly according to both the number of pseudointerfaces and by the quadrature order, thus limiting the effectiveness of the method.

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In the present work we greatly improve the efficiency of the above-mentioned method. This is accomplished by two changes. First, we recognize that the original method frequently repeated the same transport calculation; we show how to combine equivalent realizations in order to perform each unique transport calculation only once. This yields identical results in a much more efficient manner. Secondly, we recognize that many of the transport problems generated have very low weight (probability). We introduce a filtering technique to eliminate many low-weight transport problems to obtain nearly identical results at reduced cost. The combination of these two techniques allows the improved algorithm to treat problems of greater complexity than before for the same computational cost.

The rest of the paper is organized as follows. In Section 2 we briefly describe the original algorithm and then define our improvements to it. In Section 3 we present results for the improved algorithm for a set of benchmark problems. In Section 4 we present conclusions and ideas for future work.

2 ALGORITHMS

In this section we describe the original method first reported in [1]. We present both the properties of the method and its procedure. Then we define how we transform that method into a more efficient one.

2.1 Original Method

In [1] we showed that a Markovian binary stochastic medium in one-dimensional slab geometry has the following properties:

1. It may be described by regions separated by "pseudointerfaces" with an effective combined average chord length $\lambda_c = \lambda_1\lambda_2/(\lambda_1 + \lambda_2)$, where λ_1 and λ_2 are the average chord lengths of materials 1 and 2, respectively.
2. The frequency with which P pseudointerfaces occur is governed by the Poisson distribution $f(P;\lambda_c) = e^{-\lambda_c}{\lambda_c}^P/P!$.
3. The location of pseudointerfaces is uniformly distributed, and thus independent of the location of other pseudointerfaces.

The above properties allow us to decompose the problem into a set of stratified subproblems characterized by the number of pseudointerfaces. For a given number of pseudointerfaces we distribute each pseudointerface by means of a spatial quadrature rule. For each set of pseudointerface distributions we permute the materials in each spatial region to define different transport problems. The weighted sum of the transport results yields the (discretized) ensemble average.

This process is depicted for one example problem in Table I. This example corresponds to Tables 4-6 in [2] for a problem thickness of s=0.1; the material chord lengths are λ_1=9.9 and λ_2=1.1. In the first two columns we list the number of pseudointerfaces and the corresponding Poisson probability; in this case we truncate after two pseudointerfaces. For a given number of pseudointerfaces we examine each possible location of them; these locations and the corresponding probabilities are depicted in columns 3 and 4, respectively. For example, for two pseudointerfaces and a two-point quadrature there are four possible pseudointerface distributions with equal probability of 0.25. For each geometric realization depicted in column 3 there are

various material permutations (column 5) with associated probabilities (column 6). Transport calculations are performed for each problem depicted in column 5. These results are weighted by the product of the probabilities in columns 2, 4, and 6 (adjusted for the truncation of the Poisson distribution) and summed to produce an ensemble average.

Table I. Decomposition of example stochastic problem into subproblems by means of pseudointerfaces

Pseudointerfaces		Pseudointerface distribution		Material distribution		Problem
Number	Probability	Configuration	Probability	Configuration	Probability	
0	0.903924		1	1	0.9	1
				2	0.1	2
1	0.091305	1	0.5	1,1	0.81	1
				1,2	0.09	3
				2,1	0.09	4
				2,2	0.01	2
		1	0.5	1,1	0.81	1
				1,2	0.09	5
				2,1	0.09	6
				2,2	0.01	2
2	0.004611	1,2	0.25	1,1	0.81	1
				1,2	0.09	3
				2,1	0.09	4
				2,2	0.01	2
		1 2	0.25	1,1,1	0.729	1
				1,1,2	0.081	5
				1,2,1	0.081	7
				1,2,2	0.009	3
				2,1,1	0.081	4
				2,1,2	0.009	8
				2,2,1	0.009	6
				2,2,2	0.001	2
		2 1	0.25	1,1,1	0.0729	1
				1,1,2	0.081	5
				1,2,1	0.081	7
				1,2,2	0.009	3
				2,1,1	0.081	4
				2,1,2	0.009	8
				2,2,1	0.009	6
				2,2,2	0.001	2
		1,2	0.25	1,1	0.81	1
				1,2	0.09	5
				2,1	0.09	6
				2,2	0.01	2

2.2 Proposed Improvements

2.2.1 Focus on interfaces

The first of our efficiency improvements comes from recognizing that many of the transport problems generated by the above procedure are not unique. For example, in the last column of Table I we list a unique identifier for each unique transport problem; there are only 8 unique problems, whereas the original procedure would perform 34 calculations. By merging these duplicated problems together we reduce the computational burden.

Figure 1. Example problem with fifteen-point quadrature for interface locations.

Figure 2. Example realization with interface locations and material regions.

Procedurally this occurs as follows. We begin by choosing a numerical quadrature to define possible interface locations; this is graphically depicted in Figure 1. Then we loop over the possible number of interfaces, chosen based on accuracy and expense. For a given number of interfaces we examine each possible set of locations and starting material; one example is given in Figure 2. This defines a unique transport problem. To determine the weighting we loop over the possible number of pseudointerfaces (at least one per interface will be needed) to determine the Poisson weight. We implicitly loop over the various distributions of pseudointerface locations that can yield the selected distribution of interfaces, accumulating the probabilities of each permutation. As in the original method we compute the weighted sum of the transport results to obtain the ensemble average. If the quadrature weights are equal it may be shown that the probability p_T of a given transport problem T is given by

$$w_T = (wn)^p p_1^{n_1+N_{21}} p_2^{n_2+N_{12}} \frac{N_1!}{n_1!\,(N_1-n_1)!} \frac{N_2!}{n_2!\,(N_2-n_2)!} \sum_{j=0}^{n} (-1)^j \left(1-\frac{j}{n}\right)^p \frac{n!}{j!\,(n-j)!} \quad (1)$$

$$p_T = p_{m_l} \sum_{p=0}^{P_{max}} p_{Poisson} \sum_{i=0}^{p} \sum_{n_1=0}^{\min(N_1,p-i)} \sum_{n_2=0}^{\min(N_2,p-i-n_1)} w_T \quad (2)$$

where p_{m_l} is the probability of material m occurring at the left boundary of the problem, P_{max} is the maximum number of pseudointerfaces to be modeled, $p_{Poisson}$ is the Poisson probability of p pseudointerfaces, i is the number of interfaces in a given problem, n_1 and n_2 are the number of

quadrature points within materials 1 and 2 to which at least one pseudointerface is assigned, N_1 and N_2 are the number of quadrature points within materials 1 and 2, N_{12} and N_{21} are the number of interfaces with materials 1 or 2 on the left side, n is the total number of quadrature points to which at least one pseudointerface is assigned, w is the quadrature weight, and p_1 and p_2 are the probabilities of materials 1 and 2 occurring at any location.

In [1] we showed that the algorithmic complexity of the original algorithm is $O(2^{N+1}N^{P_{max}})$, where N is the number of quadrature points. It is easily shown that the modified algorithm has complexity $O(2^{N+1})$. The number of unique transport problems to be solved is depicted in Table II for a select number of quadrature points and pseudointerfaces; this does not depend on any other parameters (e.g. material statistics).

Table II. Number of unique transport problems required for given number of quadrature points and pseudointerfaces

N	P_{max}					
	1	2	3	7	11	15
3	8	14	16	16	16	16
7	16	58	128	256	256	256
11	24	134	464	3632	4096	4096
15	32	242	1152	32768	64384	65536

Table III. Number of unique transport problems required after filtering ($P_{max} = N$, benchmark problems 4-6 from [2], x=10).

N	Cumulative weight				
	0.9	0.95	0.99	0.995	0.999
3	5	7	11	14	16
7	22	42	115	135	200
11	106	250	809	1200	2092
15	333	1010	5063	7764	15871
19	883	2412	19146	34873	99275
23	2152	5884	65126	115662	477477

2.2.2 Filtering

Our second proposed change to the algorithm is to allow for problem filtering. The preceding procedure for generating realizations creates a transport problem for every possible material distribution between pseudointerfaces, even when such realizations may be quite rare. By ignoring the lowest-weight realizations we can substantially reduce the number of transport calculations without significantly degrading the quality of solution. For the purposes of this study we do this by including only the highest-weighted problems whose cumulative weight just equals or exceeds a requested threshold; all others are ignored. The remaining weights are

adjusted so that they sum to unity. The number of realizations included by this procedure depends on both the material statistics and the spatial domain size. We give an example of this reduction for a particular stochastic problem for select parameters in Table III. Comparison with Table II shows a great reduction in the number of transport problems required, even for cumulative weights approaching unity.

3 NUMERICAL RESULTS

In order to test our modified algorithm we reexamine the benchmark problems first reported in [2]. These problems consist of nine different combinations of binary media and mixing statistics for three different slab widths. The problems are monoenergetic in one-dimensional slab geometry. We restrict our attention to the "rod" problems, which use an S2 Gauss-Lobatto quadrature ($\mu = \pm 1$). The problems are driven by an isotropic flux on the left boundary. All scattering is isotropic. The reflected and transmitted currents are the transport quantities examined.

We generate the results for individual realizations with the Sceptre deterministic code [3] using its discretization of the first-order form of the linear monoenergetic Boltzmann equation, controlling the iterative errors to be less than 10^{-7} and spatial errors to be less than 10^{-6} [4]. The spatial quadrature for the interface locations is a simple bisection rule with uniform weights to create equal-sized regions. We have generated results for all cases and slab widths. This is too much data to report here, but we note that the observed errors are related to the material statistics, which are identical for cases 1-3, 4-6, and 7-9, respectively (only the cross sections differ within each of the three sets). Thus we will present results only for the first member of each set, which consists of small amounts of a strong pure scatterer mixed with a larger quantity of a weak pure absorber. We also note that the errors for all thin problems (x=0.1) were less than 1% in all but a few very coarse calculations, so will not explicitly show them either. In all cases the errors are measured with respect to the benchmarks generated by Monte Carlo sampling reported in [2], which are accurate to 0.1-1% error [2,4]. We show these results in Tables IV-XV as a function of the number of quadrature points and the maximum number of pseudointerfaces, where we also note the average number of pseudointerfaces in the undiscretized stochastic problem.

Table IV. Relative error in reflection, case 1, x=1 (P_{avg}=10.1).

N	P_{max}					
	1	2	3	7	11	15
3	-0.423	-0.325	-0.266	-0.182	-0.171	-0.170
7	-0.437	-0.325	-0.247	-0.090	-0.046	-0.039
11	-0.443	-0.330	-0.248	-0.075	-0.021	-0.011
15	-0.445	-0.333	-0.251	-0.071	-0.013	-0.003

Table V. Relative error in transmission, case 1, x=1 (P_{avg}=10.1).

N	P_{max}					
	1	2	3	7	11	15
3	0.128	0.098	0.081	0.055	0.052	0.051
7	0.133	0.099	0.075	0.027	0.014	0.012
11	0.134	0.100	0.075	0.023	0.006	0.003
15	0.135	0.101	0.076	0.022	0.004	0.001

Table VI. Relative error in reflection, case 4, x=1 (P_{avg}=1.01).

N	P_{max}					
	1	2	3	7	11	15
3	-0.03	0.02	0.02	0.03	0.03	0.03
7	-0.05	0.01	0.02	0.02	0.02	0.02
11	-0.06	< 0.01	0.01	0.01	0.01	0.01
15	-0.06	< 0.01	0.01	0.01	0.01	0.01

Table VII. Relative error in transmission, case 4, x=1 (P_{avg}=1.01).

N	P_{max}					
	1	2	3	7	11	15
3	0.005	-0.002	-0.003	-0.004	-0.004	-0.004
7	0.007	-0.001	-0.002	-0.003	-0.003	-0.003
11	0.008	< 0.001	-0.002	-0.002	-0.002	-0.002
15	0.009	0.001	-0.001	-0.002	-0.002	-0.002

Table VIII. Relative error in reflection, case 7, x=1 (P_{avg}=0.396).

N	P_{max}					
	1	2	3	7	11	15
3	0.01	0.01	0.01	0.01	0.01	0.01
7	< 0.01	< 0.01	0.01	0.01	0.01	0.01
11	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01
15	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01

Table IX. Relative error in transmission, case 7, x=1 (P_{avg}=0.396).

N	P_{max}					
	1	2	3	7	11	15
3	-0.002	-0.003	-0.003	-0.003	-0.003	-0.003
7	-0.001	-0.002	-0.002	-0.002	-0.002	-0.002
11	< 0.001	-0.001	-0.001	-0.001	-0.001	-0.001
15	< 0.001	-0.001	-0.001	-0.001	-0.001	-0.001

Table X. Relative error in reflection, case 1, x=10 (P_{avg}=101).

N	P_{max}					
	1	2	3	7	11	15
3	-0.735	-0.696	-0.671	-0.632	-0.624	-0.623
7	-0.734	-0.683	-0.643	-0.544	-0.497	-0.473
11	-0.734	-0.681	-0.636	-0.516	-0.448	-0.406
15	-0.734	-0.680	-0.634	-0.504	-0.425	-0.374

Table XI. Relative error in transmission, case 1, x=10 (P_{avg}=101).

N	P_{max}					
	1	2	3	7	11	15
3	4.7	4.4	4.2	3.8	3.8	3.8
7	4.7	4.3	4.0	3.2	2.9	2.7
11	4.7	4.3	3.9	3.0	2.5	2.3
15	4.7	4.3	3.9	3.0	2.4	2.0

Table XII. Relative error in reflection, case 4, x=10 (P_{avg}=10.1).

N	P_{max}					
	1	2	3	7	11	15
3	-0.54	-0.48	-0.43	-0.37	-0.36	-0.36
7	-0.54	-0.46	-0.39	-0.22	-0.17	-0.16
11	-0.54	-0.45	-0.37	-0.18	-0.10	-0.09
15	-0.54	-0.45	-0.37	-0.16	-0.07	-0.05

Table XIII. Relative error in transmission, case 4, x=10 (P_{avg}=10.1).

N	P_{max}					
	1	2	3	7	11	15
3	0.69	0.59	0.53	0.44	0.43	0.43
7	0.70	0.57	0.48	0.26	0.20	0.19
11	0.70	0.57	0.47	0.21	0.12	0.10
15	0.70	0.57	0.46	0.19	0.08	0.06

Table XIV. Relative error in reflection, case 7, x=10 (P_{avg}=3.96).

N	P_{max}					
	1	2	3	7	11	15
3	-0.127	-0.062	-0.033	-0.014	-0.014	-0.014
7	-0.138	-0.059	-0.023	0.004	0.005	0.005
11	-0.143	-0.061	-0.023	0.006	0.006	0.006
15	-0.146	-0.063	-0.024	0.005	0.006	0.006

Table XV. Relative error in transmission, case 7, x=10 (P_{avg}=3.96).

N	P_{max}					
	1	2	3	7	11	15
3	0.37	0.18	0.09	0.04	0.04	0.04
7	0.40	0.17	0.06	-0.01	-0.02	-0.02
11	0.42	0.18	0.07	-0.02	-0.02	-0.02
15	0.43	0.18	0.07	-0.02	-0.02	-0.02

We observe several trends in the above data:

- The errors are not monotonic in either N or P_{max} separately, but they do appear to be monotonic as both parameters increase (e.g. when N= P_{max}).
- The accuracy is inversely related to P_{avg}, degrading as the average number of pseudointerfaces increases. This is to be expected, since our discretization truncates the Poisson distribution of pseudointerfaces.
- For some of the problems (e.g. Table XV) there appears to be some error still remaining. This could be the result of statistical and/or spatial errors in the benchmarks.
- In comparing the computational cost required for 1% accuracy, we find that our method requires fewer realizations than Monte Carlo sampling [4] for x=0.1 and x=1 for the above cases, and for x=10 for case 7.

Next we examine the results of filtering. In Tables XVI and XVII we show the relative difference (not the relative error) between the results with or without filtering for case 4 and x=10. As N increases we observe that the discrepancy is approximately equal to the weight of the realizations that were filtered out, which can be a useful guide for choosing filtering parameters. Comparison of these tables with Tables III, XII, and XIII shows that we can obtain equivalent accuracy for a fraction of the cost with this technique. Alternatively, we can obtain greater accuracy for a fixed cost, as shown in Tables XVIII and XIX, where we examine greater values for N and P_{max} than we did without filtering.

Table XVI. Relative difference between filtered and unfiltered reflection, case 4, x=10 ($P_{max} = N$).

N	Cumulative weight				
	0.9	0.95	0.99	0.995	0.999
3	-0.361	-0.180	-0.044	-0.013	0
7	-0.193	-0.110	-0.023	-0.013	-0.002
11	-0.154	-0.083	-0.018	-0.010	-0.002
15	-0.149	-0.069	-0.015	-0.008	-0.002

Table XVII. Relative difference between filtered and unfiltered transmission, case 4, x=10 ($P_{max} = N$).

N	Cumulative weight				
	0.9	0.95	0.99	0.995	0.999
3	0.101	0.047	0.010	0.003	0
7	0.084	0.048	0.008	0.004	< 0.001
11	0.094	0.045	0.009	0.005	< 0.001
15	0.100	0.040	0.008	0.004	< 0.001

Table XVIII. Relative error in reflection, x=10, $P_{max} = N = 19$.

case	Cumulative weight				
	0.9	0.95	0.99	0.995	0.999
1	-0.382	-0.350	-0.323	-0.319	-0.316
4	-0.17	-0.11	-0.05	-0.04	-0.04
7	-0.006	0.002	0.004	0.005	0.005

Table XIX. Relative error in transmission, x=10, $P_{max} = N = 19$.

case	Cumulative weight				
	0.9	0.95	0.99	0.995	0.999
1	1.9	1.8	1.7	1.7	1.7
4	0.14	0.09	0.05	0.04	0.04
7	0.02	< 0.01	-0.01	-0.02	-0.02

4 CONCLUSIONS

Previously we constructed a method for approximately solving stochastic media transport problems by creating realizations through a deterministic process rather than by Monte Carlo sampling. This method focused on pseudointerfaces within the realizations and could be quite expensive due to duplicated work. In the present research we have modified the algorithm to focus on interfaces, which yields only unique transport problems. We also introduced a method to filter out low-weight realizations in order to obtain nearly the same accuracy at reduced cost. Our numerical results demonstrate that these changes make the algorithm competitive with Monte Carlo sampling for many benchmark problems. The expense of the method is governed by the average number of pseudointerfaces present in the original stochastic problem.

For future work we would like to examine more than just the rod problem. In addition to the S_{16} problems examined in [2], we would like to explore its application to multidimensional problems. Furthermore, we are interested in using it to construct improved local models, such as generalizations to the Levermore-Pomraning closure [2], in which the statistical error of Monte Carlo sampling may prove problematic. Work in this area is presented in a companion paper [5].

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