An Optimal-Cost Monte Carlo Approach to Stochastic Media Transport Calculations

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INTRODUCTION

The Monte Carlo uncertainty resulting from the stochasticity of the "brute-force" approach [1] to solving quantities of interest in stochastic media transport problems converges as the inverse of the square root of the number of realizations sampled. This convergence relationship enables projecting the uncertainty attainable as a function of the number of realizations (cost) such that the user can make informed decisions about the tradeoff between runtime and uncertainty. While useful, this model of uncertainty projection does not incorporate the error or uncertainty of deterministic or Monte Carlo transport solvers. We here propose an uncertainty model which incorporates uncertainty from the random sampling of realizations and Monte Carlo transport and use Lagrangian optimization [2] to study the relationship between computational cost and the total uncertainty. This optimal-cost Monte Carlo (OCMC) approach shows that square-root convergence can be attained (or missed) and provides equations which, along with a cheap "scoping calculation", enable selection of number of realizations and number of particle histories to most cheaply reach a desired level of uncertainty (or conversely minimize uncertainty for a set computational cost budget).

For some types of stochastic media, such as that in this paper, it is known how to sample realizations from the uncertain space such that Monte Carlo sampling of realizations may be used, but the uncertain space is not described in terms of a finite number of random variables (as in, for example, Ref. [3]) such that many other uncertainty quantification techniques may not be used. While some work is underway to describe the uncertain space in terms of a finite number of random variables [4, 5], the approach in this paper instead accepts the use of Monte Carlo sampling of realizations and seeks to optimize the overall solution process much as Multi-level Monte Carlo seeks to for problems involving deterministic physics solutions [2].

In the first section of this paper, Monte Carlo transport in binary Markovian stochastic media is briefly described. In the second section, OCMC analysis is performed for this problem and an expression for the savings against a plausible alternative parameter selection approach is derived. In the third section, the application of OCMC theory is demonstrated and the theory numerically tested.

PROBLEM DESCRIPTION

We choose purely absorbing materials and solve the following attenuation problem for transmittance on each realization:

$$\mu\frac{\partial\psi(x,\mu,\omega)}{\partial x}+\Sigma_t(x,\omega)\psi(x,\mu,\omega)=0, \tag{1a}$$

$$0\le x\le L;\quad -1\le\mu\le 1, \tag{1b}$$

$$\psi(0,\mu)=\delta(1-\mu),\ \ \mu>0;\quad \psi(L,\mu)=0,\ \ \mu<0, \tag{1c}$$

where $\psi(x,\mu,\omega)$ is angular flux, $\Sigma_t(x,\omega)$ is the total cross section, and x, μ, and ω denote spatial, angular, and stochastic dependence. Particles are normally incident on the left side of the slab with thickness L with otherwise vacuum boundary conditions. Transmittance is solved analytically for each realization when generating the benchmark solution as in Ref. [3] and using Monte Carlo particle transport (MC) otherwise. We use N to represent the number of particle histories simulated on each realization, such that the total number of particle histories simulated is $N_{tot} = RN$.

Realizations of the Markovian media are generated, as described in detail in Ref. [1], by randomly sampling successive material chords from an exponential distribution. We use R to denote the number of realizations sampled for an ensemble.

OPTIMAL-COST MONTE CARLO ANALYSIS

Uncertainty and Cost Functions

Uncertainty is introduced in these calculations in two ways. Random sampling of realizations introduces uncertainty as a function of the number of random samples, R:

$$u_{RS}=\frac{\sigma_{RS}}{\sqrt{R}}, \tag{2a}$$

where σ^2_{RS} is the sample variance. Monte Carlo transport introduces uncertainty on each realization as a function of the number of particle histories, N:

$$u_{MC,i}=\frac{\sigma_{MC,i}}{\sqrt{N}}, \tag{2b}$$

where $\sigma^2_{MC,i}$ is the variance on each realization i. These uncertainties are sometimes called by names such as the "standard error of the mean". There is about a 68% chance that the error yielded by a calculation is less than the computed uncertainty. It is seen from Eqs. (2a) and (2b) that in the limit of many realizations or histories, convergence is as the square-root of the number of samples, i.e., $u_{RS}\propto R^{-1/2}$ and $u_{MC,i}\propto N^{-1/2}$.

Monte Carlo uncertainty from each realization is propagated to the averaged quantity of interest according to the traditional approach to uncertainty propagation:

$$u^2_{MC}=\sum_{i=1}^{R}\left(\frac{1}{R}\right)^2 u^2_{MC,i}. \tag{3}$$

Monte Carlo variance is accumulated as

$$\sigma^2_{MC}=\frac{1}{R}\sum_{i=1}^{R}\sigma^2_{MC,i}. \tag{4}$$

Assuming that the random sampling and Monte Carlo uncertainties are independently generated and normally distributed, their squares are added to compute the square of the total uncertainty:

$$u^2_{tot}=u^2_{RS}+u^2_{MC}. \tag{5}$$

Expanding the total uncertainty formulation (Eq. (5)) according to the propagated Monte Carlo uncertainty (Eq. (3)), unpacking the uncertainties according to Eqs. (2a) and (2b), and substituting in the average Monte Carlo variance according to Eq. (4), the total uncertainty is

$$u_{tot} = \sqrt{\frac{\sigma_{RS}^2}{R} + \frac{\sigma_{MC}^2}{RN}}. \tag{6}$$

It is seen from Eq. (6) that if the cost is computed as the total number of histories, N_{tot}, the uncertainty is most efficiently reduced by choosing one history on each realization ($N = 1$) and converging by increasing the number of realizations R. Such a conclusion would be valid if the computational cost of constructing a realization was much smaller than the cost of simulating a particle history; this is not in general the case.

The cost function in terms of computational cost is

$$t = C_{RS}R + C_{MC}N_{tot}, \tag{7}$$

where C_{RS} is the average computational time required for each realization (i.e., creating the realization, setting up the transport solve, collecting transport results, etc.) and C_{MC} is the average computational time for a particle history.

Optimal Cost Parameter Selection and Convergence

Optimal-cost Monte Carlo (OCMC) analysis uses Lagrangian optimization to either minimize the required runtime (t) to reach an uncertainty tolerance (u_{tol}) or minimize the uncertainty (u_{tot}) for a set cost budget (t_{bud}). Each Lagrangian optimization expression consists of the quantity to be minimized and the constraint, i.e., a value equal to a tolerance:

$$\mathcal{L}_{u_{tol}}(R, N, \lambda) = t - \lambda(u_{tol} - u_{tot}) \tag{8a}$$

$$\mathcal{L}_{t_{bud}}(R, N, \lambda) = u_{tot} - \lambda(t_{bud} - t). \tag{8b}$$

For each of these expressions, the following system of equations is solved to yield the values of R and N which minimize runtime or cost under the respective constraint:

$$\frac{\partial\mathcal{L}(R, N, \lambda)}{\partial R} = 0; \quad \frac{\partial\mathcal{L}(R, N, \lambda)}{\partial N} = 0; \quad \frac{\partial\mathcal{L}(R, N, \lambda)}{\partial \lambda} = 0. \tag{9}$$

Each minimization problem yields the same relationship for the optimal choice of number of histories per realization:

$$N = \frac{\sigma_{MC}}{\sigma_{RS}}\frac{\sqrt{C_{RS}}}{\sqrt{C_{MC}}}. \tag{10}$$

We see from Eq. (10) that N is independent of uncertainty tolerance or runtime budget and the number of realizations R.

We here solve the optimal number of realizations as a function of each constraint (from Eq. (8a) and Eq. (8b)):

$$R_{u_{tol}} = \frac{\sigma_{RS}^2 + \frac{\sigma_{MC}^2}{N}}{u_{tol}^2} = \frac{\sigma_{RS}^2 + \sigma_{RS}\sigma_{MC}\frac{\sqrt{C_{MC}}}{\sqrt{C_{RS}}}}{u_{tol}^2} \tag{11a}$$

$$R_{t_{bud}} = \frac{t_{bud}}{C_{RS} + C_{MC}N} = \frac{t_{bud}}{C_{RS} + \frac{\sigma_{MC}}{\sigma_{RS}}\sqrt{C_{RS}C_{MC}}}. \tag{11b}$$

If the free parameters N and R are chosen according to the relationships in Eqs. (10)-(11b), the total uncertainty or total cost will be equal to the tolerance or budget, respectively, i.e., $u_{tot} = u_{tol}$ or $t = t_{bud}$. Noting this and solving for the total uncertainty by equating the right-hand sides of (11a) and (11b) yields the uncertainty achievable as a function of cost:

$$u_{tot} = \left(\sqrt{C_{RS}}\sigma_{RS} + \sqrt{C_{MC}}\sigma_{MC}\right)t^{-1/2}. \tag{12}$$

We note that optimal parameter selection yields square-root convergence:

$$u_{tot} \propto t^{-1/2}. \tag{13}$$

Eqs. (10)-(11b) become practical for choosing N and R and Eq. (12) becomes practical for projecting the uncertainty achievable as a function of cost if σ_{MC}, σ_{RS}, C_{RS}, and C_{MC} are known or estimated. We propose estimating these parameters using a cheap "scoping calculation". Use of a scoping calculation and choosing integer values of N and R from the decimal outputs of Eqs. (10)-(11b) is demonstrated below.

Alternative Parameter Selection and OCMC Savings

We compare the performance of optimally chosen values against a plausible alternative approach for selection of R and N in which the number of histories on each realization and the number of realizations are equal, i.e., $N = R$. The total uncertainty for this alternative case is then

$$u_{alt} = \sqrt{\frac{\sigma_{RS}^2}{R} + \frac{\sigma_{MC}^2}{R^2}}, \tag{14}$$

and the computational cost is

$$t = C_{RS}R + C_{MC}R^2. \tag{15}$$

We examine each of these expressions as R grows:

$$\lim_{R\to\infty} u_{alt} = \frac{\sigma_{RS}}{\sqrt{R}} \tag{16}$$

$$\lim_{R\to\infty} t = C_{MC}R^2 \tag{17}$$

The total uncertainty in the large-R limit is then:

$$\lim_{R\to\infty} u_{alt} = \sigma_{RS}C_{MC}^{1/4}t^{-1/4}. \tag{18}$$

We first note that the full convergence expression can be solved from Eqs. (14) and (15) and that, for at least our application problem, Eq. (18) well approximates the full expression even for small values of R. We secondly note that this approach to parameter selection yields fourth-root uncertainty convergence in the asymptotic region, much worse than the square-root Monte Carlo convergence that is already generally considered slow.

Assuming that the asymptotic convergence behavior of Eq. (18) well approximates the uncertainty convergence for our alternative parameter selection scheme, the savings of the OCMC approach as compared to this alternative approach is approximated as a ratio resulting from Eq. (18) and Eq. (12):

$$\frac{u_{alt}}{u_{opt}} \approx \left(\frac{\sigma_{RS}C_{MC}^{1/4}}{\sqrt{C_{RS}}\sigma_{RS} + \sqrt{C_{MC}}\sigma_{MC}}\right)t^{1/4}. \tag{19}$$

We note the factor by which the uncertainty is reduced increases as a function of runtime such that savings are greater for more expensive calculations.

EXAMPLE USE OF OPTIMAL-COST APPROACH

We select problem parameters from Table 10 of Ref. [1], but set scattering cross sections to zero so that the well-resolved benchmark solution can be attained more cheaply using analytic solves of transmittance. Problem parameters are listed in Table I in which Λ_i, $\Sigma_{t,j}$, and $\Sigma_{s,j}$ are the average chord length, total cross section, and scattering cross section for each material $j \in \{0, 1\}$ and L is the length of the slab.

TABLE I. Stochastic Media Problem Description

$\Lambda_0 = \frac{99}{100}$	$\Sigma_{t,0} = \frac{10}{99}$	$\Sigma_{s,0} = 0$
$\Lambda_1 = \frac{11}{100}$	$\Sigma_{t,1} = \frac{100}{11}$	$\Sigma_{s,1} = 0$
$L = 1$		

Benchmark and OCMC Scoping Calculations

The benchmark transmittance of 0.542222 ± 1.0E-5 was computed using analytic solves of transmittance on an ensemble of 10^9 realizations.

We begin OCMC application by running a scoping calculation–a relatively cheap calculation used to estimate parameters–using 100 realizations (R = 100) and 5,000 particle histories on each realization ($N = 5,000$). This scoping calculation took about 4.4 seconds and produced estimates of σ_{RS}, σ_{MC}, C_{RS}, and C_{MC} as reported in Table II. Also listed are the computed transmittance, uncertainty, and actual error of the calculation (ϵ_T, computed against the benchmark solution). All values are compared against those yielded by a 16.7 minute alternative calculation ($R = N = 10389$) described below. The scoping calculation values are shown to be reasonable when compared with the values from the more expensive calculation.

TABLE II. Scoping Calculation Results

	Scoping	Alternative
σ_{RS}	0.3301	0.3302
σ_{MC}	0.3768	0.3727
C_{RS}	1.60×10^{-4}	2.51×10^{-4}
C_{MC}	9.25×10^{-6}	8.99×10^{-6}
$T \pm u_{tot}$	0.5106 ± 0.0329	0.5456 ± 0.0032
ϵ_T	-0.0316	0.0034

Application of OCMC Theory Using Scoping Calculation Results

When using the OCMC equations (i.e., Eqs. (10)-(11b)) the user will likely want to project uncertainty and runtime in order to choose the parameters for one or a few expensive calculations. We perform many calculations using parameters chosen according to the OCMC theory and our alternative approach to validate the theory in the preceding section.

The calculations we run are labeled as alternative ("alt"), optimal ("opt"), or offset ("off") cases (with subscripts indicating the projected runtime) in Table III and defined by the input parameters R and N. Projected runtimes and uncertainties are listed in Table III. In each case the target runtime is either 10, 100, or 1000 seconds, and 50 calculations are run. Parameters R and N are chosen for the alternative cases using Eq. (18) and values from the scoping calculation, rounding to a near integer as described in the rest of this paragraph. Eq. (10), using parameters from the scoping calculation, estimates the optimal N as 4.75. An integer value for N is chosen by solving the corresponding R for each of $N = 4$ and $N = 5$ using Eq. (11b), rounding the resulting Rs up to the nearest integers, using these values and Eq. (6) to project the total uncertainty, and accepting the integer value of N which projects the smaller resulting uncertainty. To further numerically explore the relationship between cost and uncertainty, we solve "offset" cases where $N = 1$ and $N = 40$ (solving for R through Eq. (11b)).

TABLE III. Projected Runtime and Uncertainty

Case	R	N	Proj. t [s]	Proj. u_{tot}
alt_{10}	1032	1032	10	0.01028
opt_{10}	48485	5	10	0.00168
alt_{100}	3280	3280	100	0.00577
opt_{100}	484848	5	100	0.00053
alt_{1000}	10389	10389	1000	0.00324
opt_{1000}	4848478	5	1000	0.00017
off_{100a}	590841	1	100	0.00065
off_{100b}	188679	40	100	0.00077

To add confidence in our uncertainty formula, we use our benchmark solution to compute the error in the transmittance value yielded from each Monte Carlo calculation and compare against the computed uncertainty. Table IV lists for each case the average observed runtime, the average computed uncertainty, the average error yielded by the calculations, and the fraction of the calculations for which the error was less than the uncertainty. The runtimes and total uncertainties were close to the projected values listed in Table III and the error was less than the uncertainty about 68% of the time as expected for each case and for the cases as a whole (276/400 = 69%).

TABLE IV. Observed Simulation Properties

Case	Obs. t [s]	Ave. u_{tot}	Ave. ϵ_T	$\epsilon_T < u_{tot}$
alt_{10}	9.9	0.01029	0.00810	36/50
opt_{10}	10.8	0.00184	0.00128	36/50
alt_{100}	97.8	0.00578	0.00513	31/50
opt_{100}	99.2	0.00058	0.00040	38/50
alt_{1000}	979.1	0.00325	0.00294	29/50
opt_{1000}	1005.5	0.00018	0.00013	38/50
off_{100b}	95.3	0.00065	0.00055	33/50
off_{100c}	103.0	0.00079	0.00059	35/50
all	N/A	N/A	N/A	276/400

The two different convergence rates–square-root and fourth-root–can be seen in the uncertainty projection trends in Figure 1 (produced using Eqs. (12) and (18) with values from the scoping calculation). For each case, the errors resulting from individual calculations are plotted as well as the mean error and the statistical uncertainty of the mean error (resulting from 50 tests per case).

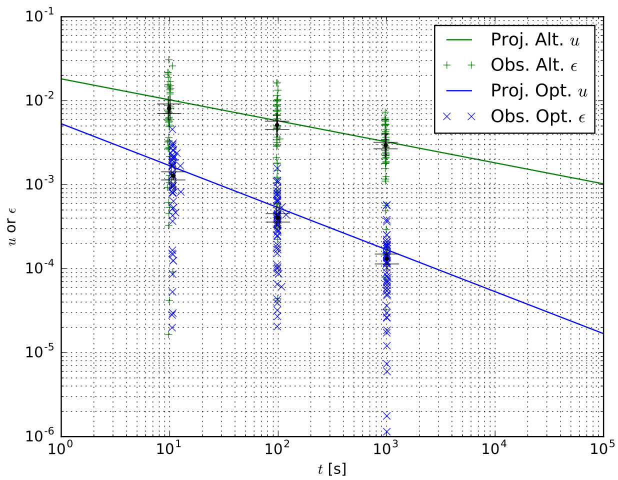

Fig. 1. Alternative and OCMC Convergence

Figure 2 shows the projected uncertainty as a function of number of histories *N* for the optimal and offset 100-second calculations as well as the error yielded by individual calculations, the average error for each case, and the uncertainty on that error. The uncertainty projection trend shows how uncertainty may be minimized with an appropriate choice of *N* and the numerically computed errors provide confidence in the uncertainty projections.

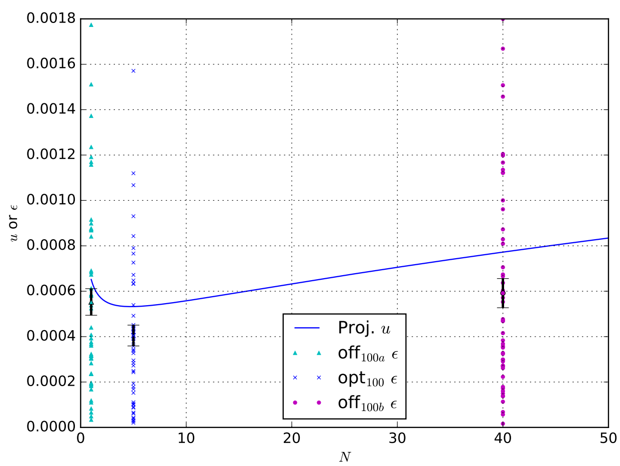

Fig. 2. Uncertainty as a Function of *N*

The projected and observed factors by which the uncertainty is reduced using OCMC parameters are shown in Table V. Savings were similar to projections.

TABLE V. Projected and Observed Savings

t	Proj. Sav.	Obs. Sav.
10	6.08	5.68
100	10.82	10.14
1000	19.24	18.06

CONCLUSIONS AND FUTURE WORK

Optimal-cost Monte Carlo (OCMC) analysis is performed on a problem involving random sampling of realizations and Monte Carlo transport. The OCMC analysis shows that with proper parameter selection the convergence of the mean expectation for a quantity of interest is square-root as opposed to the quarter-root convergence of a plausible alternative parameter selection approach. The analysis provides expressions for choosing the free parameters optimally and projecting the relationship between cost and uncertainty. Application of these tools using a scoping calculation to estimate problem-specific parameters is demonstrated and the uncertainty projections of the OCMC analysis are supported through numerical experiment.

Possible future work includes application to higher-order quantities of interest, such as transmittance standard deviation; enabling a different number of histories on each realization and solving the optimal numbers; and application to problems in which the realizations have different weights resulting from, for example, a deterministic quadrature in the random space. An adaptive algorithm could be adopted which performs successively more resolved scoping calculations–reusing data from previous, less-resolved calculations–such that the OCMC process is automated efficiently and final calculations are made using accurate scoping calculation data. Finally, this general approach could be applied to a host of other problems involving more than one source of Monte Carlo uncertainty.

ACKNOWLEDGMENTS

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.

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