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A new proof of geometric convergence for general transport problems based on sequential correlated sampling methods

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ABSTRACT

In [J. Halton, Sequential Monte Carlo, Proc. Comb. Phil. Soc. 58 (1962), J. Halton, Sequential Monte Carlo Techniques for the Solution of Linear Systems, J. Sci. Comp. 9 (1994) 213–257] Halton introduced a strategy to be used in Monte Carlo algorithms for the efficient solution of certain matrix problems. We showed in [R. Kong, J. Spanier, Sequential correlated sampling methods for some transport problems, in: Harold Niederreiter, Jerome Spanier (Eds.), Monte-Carlo and Quasi Monte-Carlo Methods 1998: Proceedings of a Conference at the Claremont Graduate University, Springer-Verlag, New York, 2000, R. Kong, J. Spanier, Error analysis of sequential Monte Carlo methods for transport problems, in: Harold Niederreiter, Jerome Spanier (Eds.), Monte-Carlo and Quasi Monte-Carlo Methods 1998: Proceedings of a Conference at the Claremont Graduate University, Springer-Verlag, New York, 2000] how Halton's method based on correlated sampling can be extended to continuous transport problems and established their geometric convergence for a family of transport problems in slab geometry. In our algorithm, random walks are processed in batches, called stages, each stage producing a small correction that is added to the approximate solution developed from the previous stages. In this paper, we demonstrate that strict error reduction from stage to stage can be assured under rather general conditions and we illustrate this rapid convergence numerically for a simple family of two dimensional transport problems.

1. Introduction

Monte Carlo (MC) simulations have provided a "gold standard" of computational support for many important problems of science and engineering that are modeled using the radiative transport equation (RTE). While initial interest about 60 years ago was focused on problems arising in nuclear design and engineering, that interest has widened greatly as computational speed and efficiency have increased and now MC methods are routinely used for many other applications. The method is used often to solve problems for which no closed form or other convenient analytic solutions are available – problems for which it may be the *only* practical solution technique.

When the MC method is applied conventionally, however, its convergence is limited by the central limit theorem to the rate $O(W^{-1/2})$, where W is the number of samples generated. This means that to obtain each new decimal digit of accuracy, the sample size must be increased about a hundredfold. Because of this slow convergence, it is not unusual for difficult Monte Carlo simulations to occupy days or even weeks of computer time to solve a single problem. Researchers have

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therefore sought faster and more efficient numerical solutions to facilitate implementation of this versatile modeling technique. Variance reduction methods have been helpful but they cannot alter the underlying slow convergence *rate* unless some sort of sequential strategy is employed.

In 1962, Halton applied Monte Carlo sequential algorithms to matrix problems (see [1,2]). In his papers, Halton applied specific variance reduction strategies successively in many stages, each of which is solved using conventional Monte Carlo methods. Under suitable conditions, the error E_m after the mth stage will be strictly bounded by the error E_{m-1} obtained in the previous stage multiplied by a constant $\lambda(W)$ that depends on the number W of random walks used in each stage and on the problem input, but not on the stage number m; i.e.,

$$E_m \leqslant \lambda(W) E_{m-1}, \tag{1}$$

E_0 being the initial error. Most importantly, with a relatively small number W of random walks, one can often achieve $\lambda(W) < 1$. Thus, after m stages, the error is bounded by

$$E_m \leqslant [\lambda(W)]^m E_0, \tag{2}$$

which characterizes geometric convergence (also called "exponential convergence" in [3,5]).

In the past 20 years, researchers, notably at Los Alamos National Laboratory and Claremont Graduate University, have explored the possibility of applying similar ideas to continuous transport problems. Booth and his co-workers at Los Alamos (see [3–6]) and Spanier and his co-workers at Claremont (see [7–11]) have adopted somewhat different approaches, but both groups have achieved geometric convergence for a number of continuous transport problems. The Claremont group also proved that convergence is geometric for a special class of model transport problems [10]. What has been lacking until now, however, is a general formulation of the theory underlying many of these methods and approaches and a more general proof of their geometric convergence. We present such a theory in this paper, establishing rigorously the conditions necessary to guarantee geometric convergence for sequential correlated sampling Monte Carlo algorithms that can be applied to a large class of continuous transport problems. In other papers, we will develop similar results for other adaptive Monte Carlo methods, all of which have been shown to produce geometric convergence.

2. General principles

In this paper, we consider continuous transport problems that are formulated as integral equations of the form

$$\Psi(P) = \mathscr{K}\Psi(P) + S(P) \tag{3}$$

where

$$\begin{aligned} &\mathscr{K}\Psi(P) \equiv \int_\Gamma K(P,Q)\Psi(Q)\mathrm{d}Q, \quad P \in \Gamma \text{ the phase space,} \\ &S(P) \geqslant 0. \end{aligned} \tag{4}$$

We assume that the kernel $K(P,Q)$ is nonnegative and that there exists a constant $M > 0$ such that $|S(P)| \leqslant M$ and $|K(P,Q)| \leqslant M$. We further assume that K satisfies either

$$\max_{P\in\Gamma} \int_\Gamma K(P,Q)\mathrm{d}Q < 1 \tag{5}$$

or

$$\max_{Q\in\Gamma} \int_\Gamma K(P,Q)\mathrm{d}P < 1, \tag{6}$$

either of which, together with (4), will ensure the existence and uniqueness of a nonnegative and bounded solution $\Psi(P)$; details may be found in [7] or in [15].

Remark. For transport equations given in the form of integro-differential equations, as long as the physical process has a positive absorption probability in the problem phase space, condition (6) is always satisfied. Weaker conditions that also suffice are discussed in [7].

For physical processes described by Eq. (3), one is often only interested in estimating a number of weighted integrals of the solution. Therefore, our task can be formulated in terms of estimating one or more integrals:

$$I \equiv \int_\Gamma \Psi(P)S^*(P)\mathrm{d}P \equiv \langle \Psi, S^* \rangle, \tag{7}$$

where $S^*(P)$ is a known function and where, without loss of generality, S^* can be assumed to be nonnegative. Thus, each continuous transport problem considered here is uniquely characterized by the known nonnegative functions $S(P), K(P,Q)$, and one or more functions $S^*(P)$. In the physical context of such a problem, S describes a known source of radiation, $K(P,Q)$ describes how random walking "particles" move from state Q to state P in the phase space Γ, and the function $S^*(P)$ incorporates

properties of a radiation detector at points P in the phase space. Appropriate boundary conditions are also imposed to guarantee that a unique solution Ψ of Eq. (3) exists.

Each Monte Carlo algorithm describes how random walks are to be generated and used to provide estimates of integrals such as I and their errors. We follow the general approach of [7] here in which a probability model that mirrors features of the physical model is constructed using a few basic ideas drawn from probability theory.

Our task is to describe a random walk process (a method for generating random walks), an (unbiased) estimating random variable defined on the space Ω of all random walks for each choice of S^* and demonstrate how the sequential application of such estimators produces accelerated Monte Carlo convergence. A great variety of random walk processes and estimating random variables is possible, each of which produces unbiased estimates of the desired weighted integrals, but all of which produce different statistical errors. For ease of exposition we examine only one such sequential method here based on the repeated use of correlated sampling, and one specific type of random variable, the so-called collision estimator (see [7]). However, other sequential methods and estimators can be treated in analogous fashion. This flexibility is very useful in the design of effective and efficient MC methods, for which one needs to strike a proper balance between computational speed and accuracy, since both are involved in estimating the overall computational efficiency of the method.

The random walk process is defined by selecting a pair of nonnegative functions $\{\widehat{S}(P), \widehat{K}(P,Q)\}$ subject to the conditions:

$$\begin{aligned} &\int_\Gamma \widehat{S}(P)\mathrm{d}P = 1 \quad \text{and} \\ &\int_\Gamma \widehat{K}(P,Q)\mathrm{d}Q = 1 - \hat{p}(P) > 0. \end{aligned} \tag{8}$$

The function $\widehat{S}$ will be used to generate initial states P_0 in the phase space, while $\widehat{K}$ will be used to produce successor states Q conditioned by the current state P and the function $\hat{p}(P)$ describes the probability of terminating a random walk in state P. These functions determine random variables on the phase space Γ by means of

$$\begin{aligned} &\xi_0 \sim \widehat{S}(Q), \\ &\xi_n|\xi_{n-1} \sim \frac{\widehat{K}(\xi_{n-1},Q)}{1-\hat{p}(\xi_{n-1})}, \\ &\eta_Q \sim B(\hat{p}(Q)) : P(\eta = 1) = \hat{p}(Q), \quad P(\eta = 0) = 1 - \hat{p}(Q) \end{aligned} \tag{9}$$

where $B(\hat{p}(Q))$ is a binomial random variable and where the symbol $\xi \sim f(Q)$ means that ξ is sampled from the probability density function $f(Q), Q \in \Gamma$. Then we define random variables ζ and ω on the space Ω of all random walks $(\xi_0, \xi_1|\xi_0, \ldots, \xi_k|\xi_{k-1}, \ldots)$ by

$$\begin{aligned} \zeta &= \frac{S^*(\xi_0)}{\widehat{S}(\xi_0)} S(\xi_0) + \frac{S^*(\xi_0)}{\widehat{S}(\xi_0)} \frac{K(\xi_0,\xi_1|\xi_0)}{\widehat{K}(\xi_0,\xi_1|\xi_0)} S(\xi_1)(1-\eta_{\xi_0}) + \cdots + \frac{S^*(\xi_0)}{\widehat{S}(\xi_0)} \frac{K(\xi_0,\xi_1|\xi_0)}{\widehat{K}(\xi_0,\xi_1|\xi_0)} \cdots \frac{K(\xi_{n-1},\xi_n|\xi_{n-1})}{\widehat{K}(\xi_{n-1},\xi_n|\xi_{n-1})} S(\xi_n)(1-\eta_{\xi_0})\cdots(1-\eta_{\xi_{n-1}}) + \cdots \\ &= \frac{S^*(\xi_0)}{\widehat{S}(\xi_0)} \omega(\xi_0) \end{aligned} \tag{10}$$

where

$$\omega(\xi_0) = S(\xi_0) + \frac{K(\xi_0,\xi_1|\xi_0)}{\widehat{K}(\xi_0,\xi_1|\xi_0)} S(\xi_1)(1-\eta_{\xi_0}) + \cdots + \frac{K(\xi_0,\xi_1|\xi_0)}{\widehat{K}(\xi_0,\xi_1|\xi_0)} \cdots \frac{K(\xi_{n-1},\xi_n|\xi_{n-1})}{\widehat{K}(\xi_{n-1},\xi_n|\xi_{n-1})} S(\xi_n)(1-\eta_{\xi_0})\cdots(1-\eta_{\xi_{n-1}}) + \cdots \tag{11}$$

Notice that the estimators defined by (10) and (11) are collision estimators in the language of [7], meaning that they produce nonzero tallies for each collision point. Use of other estimating random variables, such as terminal and track length estimators [7], can also be accommodated with modest alterations in the theory.

We next describe how to make use of the random variables defined above by (10) and (11). Assume that we want to estimate the integral I defined by (7). The initial step is to choose the function pairs $\{\widehat{S}(P), \widehat{K}(P,Q)\}$ to satisfy (8). We initialize the estimation $\widetilde{I}$ of I by

$$\widetilde{I} = 0.$$

Next we outline the sampling/estimation procedure by tracing one random walk. The starting state space vector P_0 (which represents an initial collision point) is sampled from $\widehat{S}(P)$ and the contribution recorded from this event is

$$\widetilde{I} = \widetilde{I} + \frac{S^*(P_0)}{\widehat{S}(P_0)} S(P_0).$$

We then check for absorption at P_0 using the absorption probability at that vector:

$$\hat{p}(P_0) = 1 - \int_\Gamma \widehat{K}(P_0,Q)\mathrm{d}Q.$$

If the random walk is absorbed, we continue to the next random walk. Assume that the random walk is scattered at P_0. We then sample the next collision point P_1 from

$$\frac{\widehat{K}(P_0,P)}{1-\hat{p}(P_0)}$$

and record the contribution from it as

$$\widetilde{I}=\widetilde{I}+\frac{S^*(P_0)}{\widehat{S}(P_0)}\frac{K(P_0,P_1)}{\widehat{K}(P_0,P_1)}S(P_1).$$

We check again for absorption at P_1 using the absorption probability

$$\hat{p}(P_1)=1-\int_\Gamma \widehat{K}(P_1,Q)\mathrm{d}Q.$$

This process can be repeated until the random walk is terminated either through absorption or leaving the phase space domain. Generally, if the random walk encounters collisions at $P_0,P_1,\ldots,P_k$, the final contribution from the random variable we have defined is

$$\widetilde{I}=\widetilde{I}+\frac{S^*(P_0)}{\widehat{S}(P_0)}\frac{K(P_0,P_1)}{\widehat{K}(P_0,P_1)}\cdots\frac{K(P_{k-1},P_k)}{\widehat{K}(P_{k-1},P_k)}S(P_k).$$

After we have generated all of the random walks, we compute the average of $\widetilde{I}$ over the total number of random walks to obtain a final estimate of the integral I. Second moment estimates are obtained in a similar manner and the variance is determined in the usual way from these estimates of the mean and the second moment.

Concerning this algorithm we have

Theorem 1. *Assume that $P\in\Gamma$ is a fixed but arbitrary point of phase space and that $\omega(P)$ and ζ are defined by (11) and (10), respectively with $\xi_0=P$. Then,*

$$E[\omega(P)]=\Psi(P), \tag{12}$$

and

$$E[\zeta]=I. \tag{13}$$

Proof. Focusing on the general term $\omega_n(P)$ of the expression for $\omega(P)$ we calculate

$$\begin{aligned}E[\omega_n(P)]&=E\left[\frac{K(P,\xi_1|\xi_0=P)}{\widehat{K}(P,\xi_1|\xi_0=P)}\cdots\frac{K(\xi_{n-1},\xi_n|\xi_{n-1})}{\widehat{K}(\xi_{n-1},\xi_n|\xi_{n-1})}S(\xi_n)(1-\eta_P)\cdots(1-\eta_{\xi_{n-1}})\right]\\&=\int_\Gamma\frac{\widehat{K}(P,P_1)}{\int_\Gamma\widehat{K}(P,P')\mathrm{d}P'}\mathrm{d}P_1\cdots\int_\Gamma\frac{\widehat{K}(P_{n-1},P_n)}{\int_\Gamma\widehat{K}(P_{n-1},P')\mathrm{d}P'}\mathrm{d}P_n\cdot\frac{K(P,P_1)}{\widehat{K}(P,P_1)}\cdots\frac{K(P_{n-1},P_n)}{\widehat{K}(P_{n-1},P_n)}S(P_n)\cdot(1-\hat{p}(P))(1-\hat{p}(P_1))\cdots(1-\hat{p}(P_{n-1})).\end{aligned}$$

Using (8), this reduces to

$$\int_\Gamma K(P,P_1)\mathrm{d}P_1\int_\Gamma K(P_1,P_2)\mathrm{d}P_2\cdots\int_\Gamma K(P_{n-1},P_n)S(P_n)\mathrm{d}P_n,$$

which is exactly the general term of the Neumann series expression of the solution $\Psi(P)$.

As for (13), from (11) we have

$$E[\zeta]=E\left[\frac{S^*(P)}{\widehat{S}(P)}\omega(P)\right]=\int_\Gamma\frac{S^*(P)}{\widehat{S}(P)}E[\omega(P)]\widehat{S}(P)\mathrm{d}P=\int_\Gamma S^*(P)\Psi(P)\mathrm{d}P=I.$$

proving (13). □

To prove geometric convergence we will need to establish relationships between the variances of our estimators in successive stages. This can be done by making use of transport-like equations for the variances and using these to relate the variance after the mth sequential stage to that of the previous stage. The final step in our proof involves applying Tchebycheff's inequality to the random variables responsible for the estimates. We will state the needed results here, leaving the detailed proof for Appendix.

Theorem 2. *The variance of $\omega(P)$, $V_\omega[\omega(P)]$ satisfies*

$$V_\omega[\omega(P)]+(\Psi(P))^2=\int_\Gamma\left(\frac{K(P,Q)}{\widehat{K}(P,Q)}\right)^2\{V_\omega[\omega(Q)]+(\Psi(Q))^2\}\widehat{K}(P,Q)\mathrm{d}Q+(\Psi(P))^2-(\Psi(P)-S(P))^2, \tag{14}$$

and the variance of ζ, $V_\zeta[\zeta]$, can be obtained by

$$V_\zeta[\zeta] + \langle \Psi, S^* \rangle^2 = \int_\Gamma \left(\frac{S^*(P)}{\widehat{S}(P)} \right)^2 \{ V_\omega[\omega(P)] + (\Psi(P))^2 \} \widehat{S}(P) \mathrm{d}P \tag{15}$$

A sketch of the argument needed to prove this result can be more easily recognized perhaps by examining the second moment of the estimator instead of the variance. Since $\Psi(P) = E[\omega(P)]$ by Theorem 1, Eq. (14) is equivalent to the transport equation for the second moment:

$$M_\omega^2[\omega(P)] = \int_\Gamma \left(\frac{K(P,Q)}{\widehat{K}(P,Q)} \right)^2 M_\omega^2[\omega(Q)] \widehat{K}(P,Q) \mathrm{d}Q + (\Psi(P))^2 - (\Psi(P) - S(P))^2 \tag{16}$$

This equation is very plausible because the source term represents the expected square of the direct contribution from terminations at the initial state P selected, while the integral term represents the expected square of all other contributions resulting from terminations at states Q beyond the initial state. To see the latter point more clearly, rewrite (16) as

$$M_\omega^2[\omega(P)] = \int_\Gamma (1 - \hat{p}(P)) \left(\frac{K(P,Q)}{\widehat{K}(P,Q)} \right)^2 M_\omega^2[\omega(Q)] \frac{\widehat{K}(P,Q)}{\int \widehat{K}(P,Q) \mathrm{d}Q} \mathrm{d}Q + (\Psi(P))^2 - (\Psi(P) - S(P))^2$$

so that the integral term is more easily recognized as requiring continuation of the random walk beyond its initial state, P. As we will see in Appendix, a complete proof of results such as (14) requires making repeated use of the relationships linking unconditional and conditional means and variances, which leads to the Neumann series representation for the solution of (14).

3. Sequential correlated sampling methods

In this section, we construct a sequential correlated sampling MC algorithm using the estimators developed in the previous section. As we mentioned earlier, a similar algorithm was first used by Halton [1] in 1962 to solve discrete transport (matrix) problems.

To solve Eq. (3), we begin with an initial guess $\tilde{\psi}^0(P)$ of the solution at P (which could be taken to be zero) and then introduce a first correction $\psi^1(P)$ by setting

$$\Psi(P) = \tilde{\psi}^0(P) + \psi^1(P). \tag{17}$$

Substituting (17) into (3) produces an equation for $\psi^1(P)$

$$\psi^1(P) = K\psi^1(P) + S^1(P), \tag{18}$$

where

$$S^1(P) = S(P) - \tilde{\psi}^0(P) + K\tilde{\psi}^0(P). \tag{19}$$

Applying conventional Monte Carlo methods to (18) produces an approximate solution $\tilde{\psi}^1(P)$.

Assuming that we have obtained $\tilde{\psi}^1(P)$, $\tilde{\psi}^2(P), \ldots, \tilde{\psi}^{m-1}(P)$, introduce a new function $\psi^m(P)$ by setting

$$\Psi(P) = \tilde{\psi}^0(P) + \tilde{\psi}^1(P) + \cdots + \tilde{\psi}^{m-1}(P) + \psi^m(P). \tag{20}$$

Substituting (20) into (3) then produces an equation for the mth stage correction $\psi^m(P)$

$$\psi^m(P) = K\psi^m(P) + S^m(P), \tag{21}$$

where

$$S^m(P) = S^{m-1}(P) - \tilde{\psi}^{m-1}(P) + K\tilde{\psi}^{m-1}(P) = S(P) - \widetilde{\Psi}^{m-1}(P) + K\widetilde{\Psi}^{m-1}(P), \tag{22}$$

and where

$$\widetilde{\Psi}^{m-1}(P) = \tilde{\psi}^0(P) + \tilde{\psi}^1(P) + \cdots + \tilde{\psi}^{m-1}(P). \tag{23}$$

Applying conventional Monte Carlo methods to (21) produces an approximate solution $\tilde{\psi}^m(P)$.

Repeating this recursive process produces a sequence of approximations $\widetilde{\Psi}^1(P), \ldots, \widetilde{\Psi}^m(P)$ to $\Psi(P)$. It is then natural to ask: does this sequence converge to the true solution $\Psi(P)$? If so, what is the convergence rate? In this section, we will give a positive answer to the first question, and prove that the convergence is actually geometric.

Theorem 3. *Assume that either (5) or (6) is satisfied, and that the phase space Γ has finite Lebesgue measure; i.e., there is a constant κ_Γ such that*

$$\kappa_\Gamma \equiv \mathrm{meas}[\Gamma] < \infty. \tag{24}$$

Then for any $\varepsilon > 0$ and $\lambda < 1$, there is a threshold number, W_0, of random walks per adaptive stage, such that when at least W_0 random walks are generated in each adaptive stage,

$$\Pr\{\sup_{P\in\Gamma}|\Psi(P) - \widetilde{\Psi}^m(P)| \leqslant \lambda \sup_{P\in\Gamma}|\Psi(P) - \widetilde{\Psi}^{m-1}(P)|\} > 1 - \varepsilon. \tag{25}$$

The integer W_0 is independent of the stage number m.

Proof. First, we connect $\Psi(P) - \widetilde{\Psi}^m(P)$ to the solution for each stage. According to (20), we have

$$\begin{aligned}\Psi(P) - \widetilde{\Psi}^m(P) &= (\tilde{\psi}^0(P) + \tilde{\psi}^1(P) + \cdots + \tilde{\psi}^{m-1}(P) + \psi^m(P)) - (\tilde{\psi}^0(P) + \tilde{\psi}^1(P) + \cdots + \tilde{\psi}^{m-1}(P) + \tilde{\psi}^m(P)) \\ &= \psi^m(P) - \tilde{\psi}^m(P).\end{aligned} \tag{26}$$

Now, we apply (15) of Theorem 2 to Eq. (21).

$$V_\omega[\omega^m(P)] + (\psi^m(P))^2 = \int_\Gamma \frac{(K(P,Q))^2}{\widehat{K}(P,Q)}(V_\omega[\omega^m(Q)] + (\psi^m(Q))^2)\mathrm{d}Q + (\psi^m(P))^2 - (\psi^m(P) - S^m(P))^2. \tag{27}$$

Notice that

$$|(\psi^m(P))^2 - (\psi^m(P) - S^m(P))^2| = |2\psi^m(P)S^m(P) - (S^m(P))^2| \leqslant \delta(\psi^m(P))^2 + \left(1 + \frac{1}{\delta}\right)(S^m(P))^2$$

for any $\delta > 0$ (to be determined). We have

$$V_\omega[\omega^m(P)] + (\psi^m(P))^2 \leqslant \int_\Gamma \frac{(K(P,Q))^2}{\widehat{K}(P,Q)}(V_\omega[\omega^m(Q)] + (\psi^m(Q))^2)\mathrm{d}Q + \delta(\psi^m(P))^2 + \left(1 + \frac{1}{\delta}\right)(S^m(P))^2. \tag{28}$$

At this point, we make use of the results in Theorem 1 of [15]. Since the function $\widehat{K}(P,Q)$ is at our disposal, we may assume that $\widehat{K}(P,Q)$ satisfies either

$$\max_{P\in\Gamma}\int_\Gamma \frac{(K(P,Q))^2}{\widehat{K}(P,Q)}\mathrm{d}Q < 1,$$

or

$$\max_{Q\in\Gamma}\int_\Gamma \frac{(K(P,Q))^2}{\widehat{K}(P,Q)}\mathrm{d}P < 1.$$

For example, because of either (5) or (6) we can simply pick $\widehat{K}(P,Q) = K(P,Q)$.

Now, according to Theorem 1 of [15], there is a constant C_1, only depending on the kernel and the size of the phase space Γ, such that

$$V_\omega[\omega^m(P)] + (\psi^m(P))^2 \leqslant C_1 \sup_{P\in\Gamma}(\delta(\psi^m(P))^2 + \left(1 + \frac{1}{\delta}\right)(S^m(P))^2). \tag{29}$$

Now, we can choose δ such that $C_1\delta < 1$. We then have

$$V_\omega[\omega^m(P)] \leqslant C_1\left(1 + \frac{1}{\delta}\right)\sup_{P\in\Gamma}(S^m(P))^2.$$

According to (22), we have

$$\begin{aligned}|S^m(P)| &= |S(P) - \widetilde{\Psi}^{m-1}(P) + K\widetilde{\Psi}^{m-1}(P)| = |\Psi(P) - \widetilde{\Psi}^{m-1}(P) - K(\Psi(P) - \widetilde{\Psi}^{m-1}(P))| \\ &\leqslant |\Psi(P) - \widetilde{\Psi}^{m-1}(P)| + \left|\int_\Gamma K(P,Q)(\Psi(Q) - \widetilde{\Psi}^{m-1}(Q))\mathrm{d}Q\right|.\end{aligned} \tag{30}$$

Combining (29) and (30) produces

$$\begin{aligned}V_\omega[\omega^m(P_0)] + (\psi^m(P_0))^2 &\leqslant C_1\left(1 + \frac{1}{\delta}\right)\sup_{P\in\Gamma}\left(|\Psi(P) - \widetilde{\Psi}^{m-1}(P)| + \left|\int_\Gamma K(P,Q)(\Psi(Q) - \widetilde{\Psi}^{m-1}(Q))\mathrm{d}Q\right|\right)^2 \\ &\leqslant \left(C_1\left(1 + \frac{1}{\delta}\right)\sup_{P\in\Gamma}\left(1 + \left|\int_\Gamma K(P,Q)\mathrm{d}Q\right|\right)^2\right)\sup_{P\in\Gamma}\left|\Psi(P) - \widetilde{\Psi}^{m-1}(P)\right|^2 \\ &= C_2\sup_{P\in\Gamma}|\Psi(P) - \widetilde{\Psi}^{m-1}(P)|^2,\end{aligned} \tag{31}$$

where

$$C_2 = C_1\left(1 + \frac{1}{\delta}\right)\sup_{P\in\Gamma}\left(1 + \left|\int_\Gamma K(P,Q)\mathrm{d}Q\right|\right)^2.$$

Now, by Tchebycheff's inequality, for W samples of $\omega^m(P)$ and any $\varepsilon > 0$,

$$P\left\{|\psi^m(P) - \tilde{\psi}^m(P)| \leqslant \sqrt{\frac{V_\omega[\omega^m(P)]}{\varepsilon W}}\right\} > 1 - \varepsilon,$$

or by (26),

$$P\left\{|\Psi(P) - \widetilde{\Psi}^m(\xi_0)| \leqslant \sqrt{\frac{V_\omega[\omega^m(P)]}{\varepsilon W}}\right\} > 1 - \varepsilon. \tag{32}$$

Combining (31) and (32) produces

$$P\left\{|\Psi(P) - \widetilde{\Psi}^m(P)| \leqslant \sqrt{\frac{C_2}{\varepsilon W}}\sup_{\xi_0 \in \Gamma}|\Psi(P) - \widetilde{\Psi}^{m-1}(P)|\right\} > 1 - \varepsilon,$$

which implies (25) if we choose

$$W \geqslant \frac{C_2}{\varepsilon\lambda^2}.$$

This completes the proof of Theorem 3. □

The random variables $\omega^m(P)$ can be used to approximate the solution pointwise. However, we are often interested in representing the solution everywhere as a sum of basis functions. In the rest of this section, we will adopt this point of view. We will obtain an estimate similar to that in Theorem 3. Additional details can be found in [10].

To solve (21) for $\psi^m(P)$, we assume that the solution and our approximations to it can be represented in the form

$$\Psi(P) = \sum_{i=0}^{\infty} a_i f_i(P), \tag{33}$$

where $\{f_i(P)\}_{i=0}^{\infty}$.form a complete set of orthonormal basis functions on the phase space Γ. For later convenience, we assume that there is a finite number B such that

$$\max_{P\in\Gamma}|f_i(P)| \leqslant B. \tag{34}$$

Assume that the solution $\psi^m(P)$ of (21) has the form

$$\psi^m(P) = \sum_{i=0}^{\infty} b_i^m f_i(P). \tag{35}$$

Orthonormality produces

$$b_i^m = \int_\Gamma \psi^m(P) f_i(P)\mathrm{d}P. \tag{36}$$

We now use ζ, defined by (10), to estimate all the coefficients b_i for i up to a large and fixed integer N. Assume that we have chosen $\{\widehat{S}(P), \widehat{K}(P,Q)\}$ satisfying (8). For each i, we can then define

$$\zeta_i^m = \frac{f_i(\xi_0)}{\widetilde{S}(\xi_0)}\omega^m(\xi_0), \tag{37}$$

where $\omega^m(P_0)$ is defined by (11) with $S(P)$ replaced by $S^m(P)$, defined by (22). Then, according to Theorem 1,

$$\begin{aligned} &E[\omega^m(P_0)] = \psi^m(P) \\ &E[\zeta_i^m] = b_i^m, \end{aligned} \tag{38}$$

so we can use ζ_i^m to estimate each of the coefficients b_i^m. Assume that the estimated values of b_i^m are $\tilde{b}_i^m$ and define

$$\tilde{a}_i^m = \sum_{k=0}^{m} \tilde{b}_i^k, \tag{39}$$

where we have assumed that the initial guess $\widetilde{\Psi}^0(P)$ has the form

$$\widetilde{\Psi}^0(P) = \sum_{i=0}^{N} \tilde{b}_i^0 f_i(P). \tag{40}$$

Then, the estimated solution $\widetilde{\Psi}^m(P)$ can be written as

$$\widetilde{\Psi}^m(P) = \sum_{i=0}^{N} \tilde{a}_i^m f_i(P). \tag{41}$$

Theorem 4. *Assume that either (5) or (6) is satisfied, and that the phase space Γ has finite measure, i.e., there is a number κ_Γ such that*

$$\kappa_\Gamma \equiv \text{meas}[\Gamma] < \infty. \tag{42}$$

Then for any $\varepsilon > 0$ and $\lambda < 1$, there exists a sufficiently large integer W_0 which does not depend on m, such that

$$P\left\{\sup_{P\in\Gamma}|\Psi(P) - \widetilde{\Psi}^m(P)| < \frac{C_4}{\sqrt{W_0}}\sup_{P\in\Gamma}|\Psi(P) - \widetilde{\Psi}^{m-1}(P)| + \sup_{P\in\Gamma}|r_N|\right\} \geqslant 1-\varepsilon, \tag{43}$$

where

$$r_N(P) \equiv \sum_{i=N+1}^{\infty} b_i f_i(P). \tag{44}$$

Remark. According to (20),

$$\sum_{i=N+1}^{\infty} b_i f_i(P) = \sum_{i=N+1}^{\infty} a_i f_i(P). \tag{45}$$

Thus, we can choose N so large that $r_N(P)$ is no more than any error level that we prescribe. Therefore, (43) expresses geometric convergence with a small error modification that is caused by the truncation of the infinite series expansion.

Proof. For each i, we can follow the proof of Theorem 3 to arrive at

$$V_\omega[\omega^m(P_0)] \leqslant C_1 \sup_{P\in\Gamma}(S^m(P))^2, \tag{46}$$

where the constant C_1 does not depend on stage index m. Now, according to Eq. (15)

$$\begin{aligned} V_\zeta[\zeta_i^m] &= \int_\Gamma \left(\frac{f_i(P)}{\widehat{S}(P)}\right)^2 V_\omega[\omega^m(P)]\widehat{S}(P)\mathrm{d}P + \int_\Gamma \left(\frac{f_i(P)}{\widehat{S}(P)}\right)^2 (\psi^m(P))^2\widehat{S}(P)\mathrm{d}P - \langle\psi^m, f_i\rangle^2 \\ &\leqslant C_1\int_\Gamma \frac{(f_i(P))^2}{\widehat{S}(P)}(V_\omega[\omega^m(P)] + (\psi^m(P))^2)\mathrm{d}P \leqslant C_2 \sup_{P\in\Gamma}(S^m(P))^2, \end{aligned} \tag{47}$$

where we have used the orthonormality of the basis set $\{f_i(P)\}_{i=0}^\infty$ and

$$C_2 = \sup_{P\in\Gamma}\frac{C_1}{\widehat{S}(P)}.$$

Therefore, using (30), we obtain

$$\begin{aligned} V_\zeta[\zeta_i^m] &\leqslant C_2 \sup_{P\in\Gamma}\left(|\Psi(P) - \widetilde{\Psi}^{m-1}(P)| + \left|\int_\Gamma K(P,Q)\left(\Psi(Q) - \widetilde{\Psi}^{m-1}(Q)\right)\mathrm{d}Q\right|\right)^2 \\ &\leqslant \left(C_2 \sup_{P\in\Gamma}\left(1 + \left|\int_\Gamma K(P,Q)\mathrm{d}Q\right|\right)^2\right)\sup_{P\in\Gamma}|\Psi(P) - \widetilde{\Psi}^{m-1}(P)|^2 \leqslant C_3 \sup_{P\in\Gamma}|\Psi(P) - \widetilde{\Psi}^{m-1}(P)|^2. \end{aligned} \tag{48}$$

On the other hand, according to (20) and (23), we have

$$\begin{aligned} \Psi(P) - \widetilde{\Psi}^m(P) &= \psi^m(P) - \tilde{\psi}^m(P) = \sum_{i=0}^{\infty} b_i^m f_i(P) - \sum_{i=0}^{N}\tilde{b}_i^m f_i(P) = \sum_{i=0}^{N}(b_i^m - \tilde{b}_i^m)f_i(P) + \sum_{i=N+1}^{\infty} b_i f_i(P) \\ &= \sum_{i=0}^{N}(b_i^m - \tilde{b}_i^m)f_i(P) + r_N(P), \end{aligned} \tag{49}$$

where the truncation error $r_N(P)$ can be made as small as we want upon choosing a large N. We then have

$$|\Psi(P) - \widetilde{\Psi}^m(P)| \leqslant \sum_{i=0}^{N}|b_i^m - \tilde{b}_i^m||f_i(P)| + |r_N(P)| \leqslant B\sum_{i=0}^{N}|b_i^m - \tilde{b}_i^m| + |r_N(P)|. \tag{50}$$

According to Tchebycheff's inequality, for any $\varepsilon_i > 0$,

$$P\left\{\left|b_i^m - \tilde{b}_i^m\right| < \sqrt{\frac{V_\zeta[\zeta_i^m]}{\varepsilon_i W}}\right\} \geqslant 1 - \varepsilon_i. \tag{51}$$

Using (48), we obtain

$$P\left\{|b_i^m - \tilde{b}_i^m| < \sqrt{\frac{C_3}{\varepsilon_i W}} \sup_{P\in\Gamma} |\Psi(P) - \widetilde{\Psi}^{m-1}(P)|\right\} \geqslant 1 - \varepsilon_i. \tag{52}$$

Thus, combining (50) with (52) produces

$$P\left\{|\Psi(P) - \widetilde{\Psi}^m(P)| < \frac{C_4}{\sqrt{W}} \sup_{P\in\Gamma} |\Psi(P) - \widetilde{\Psi}^{m-1}(P)| + \sup_{P\in\Gamma} |r_N|\right\} \geqslant \prod_{i=0}^{N}(1-\varepsilon_i), \tag{53}$$

where

$$C_4 = B\sqrt{C_3}\left(\sum_{i=0}^{N}\frac{1}{\varepsilon_i}\right)^{\frac{1}{2}}. \tag{54}$$

Now, for any $\varepsilon > 0$, we choose $\varepsilon_i > 0$, so that

$$\prod_{i=0}^{N}(1-\varepsilon_i) \geqslant 1 - \varepsilon. \tag{55}$$

Then, choose W_0 such that

$$W_0 \geqslant \left(\frac{C_4}{\lambda}\right)^2. \tag{56}$$

For such a W_0, we have

$$P\left\{\sup_{P\in\Gamma}|\Psi(P) - \widetilde{\Psi}^m(P)| < \frac{C_4}{\sqrt{W_0}} \sup_{P\in\Gamma} |\Psi(P) - \widetilde{\Psi}^{m-1}(P)| + \sup_{P\in\Gamma} |r_N|\right\} \geqslant 1 - \varepsilon. \tag{57}$$

The proof is completed. □

The two theorems in this section not only show that the sequence $\{\widetilde{\Psi}^m(P)\}_{m=0}^{\infty}$ is convergent, but also shows that the convergence is geometric, at least in a probabilistic sense.

Remark. The theory just presented establishes the existence of an integer W_0 such that our adaptive algorithm will converge geometrically provided that W_0 independent random walks are processed in each adaptive stage. It is, of course, of interest to determine the smallest value for W_0 that satisfies the error constraints of the transport problem under study. However, this is not easily found through the application of our very general theorems, which are intended only to establish the existence of a minimal W_0. In fact, the final step in our argument makes use of Tchebycheff's inequality, which, because it is completely general, provides extremely conservative estimates of the constants needed to determine W_0 accurately. In practice, much smaller numbers of random walks per stage will suffice to produce geometric convergence. We discuss this issue more fully in the next section.

4. Model two dimensional transport problems

To illustrate the theory developed in the previous sections, we consider the coupled system of ordinary differential equations

$$\begin{cases} \frac{\partial\psi_1}{\partial x} + \sum_t(x,y)\psi_1(x,y) = \sum_s(x,y)\sum_{j=1}^{4} p_{1j}\psi_j(x,y) + s_1(x,y), \\ -\frac{\partial\psi_2}{\partial x} + \sum_t(x,y)\psi_2(x,y) = \sum_s(x,y)\sum_{j=1}^{4} p_{2j}\psi_j(x,y) + s_2(x,y), \\ \frac{\partial\psi_3}{\partial y} + \sum_t(x,y)\psi_3(x,y) = \sum_s(x,y)\sum_{j=1}^{4} p_{3j}\psi_j(x,y) + s_3(x,y), \\ -\frac{\partial\psi_4}{\partial y} + \sum_t(x,y)\psi_4(x,y) = \sum_s(x,y)\sum_{j=1}^{4} p_{4j}\psi_j(x,y) + s_4(x,y), \end{cases} \tag{58}$$

where

$$0 < x < a, \quad 0 < y < b,$$

$$\psi_1(0,y) = Q_1(y), \quad \psi_2(a,y) = Q_2(y),$$

$$\psi_3(x,0) = Q_3(x), \quad \psi_4(x,b) = Q_4(y),$$

and where we assume

$$\sum_{j=1}^{4} p_{ji} = 1, \quad i = 1,2,3,4. \tag{59}$$

This system describes a transport problem in a rectangle R: $0 < x < a$, $0 < y < b$, and the functions $\psi_1(x,y)$, $\psi_2(x,y)$, $\psi_3(x,y)$ and $\psi_4(x,y)$ are the right, left, up and down moving fluxes, respectively.

This problem specializes to one dimensional transport on horizontal and vertical lines when the equations are suitably decoupled and the resulting decoupled system can be easily solved analytically. Thus, this family of problems plays a very useful role in debugging Monte Carlo codes such as the one developed from the algorithm described in this paper. The four boundary conditions characterize the flux incident on the boundaries of the rectangle from the exterior and prescribe a unique solution of the system (58) [17].

The system (58) can be written in matrix form by setting

$$K \equiv \sum_s (x,y) \begin{pmatrix} p_{11} & p_{12} & p_{13} & p_{14} \\ p_{21} & p_{22} & p_{23} & p_{24} \\ p_{31} & p_{32} & p_{33} & p_{34} \\ p_{41} & p_{42} & p_{43} & p_{44} \end{pmatrix}, \tag{60}$$

$$D \equiv \begin{pmatrix} \frac{\partial}{\partial x} & & & \\ & -\frac{\partial}{\partial x} & & \\ & & \frac{\partial}{\partial y} & \\ & & & -\frac{\partial}{\partial y} \end{pmatrix}, \tag{61}$$

$$\sum \equiv \begin{pmatrix} \sum_t (x,y) & & & \\ & \sum_t (x,y) & & \\ & & \sum_t (x,y) & \\ & & & \sum_t (x,y) \end{pmatrix}, \tag{62a}$$

$$S(x,y) \equiv \begin{pmatrix} s_1(x,y) \\ s_2(x,y) \\ s_3(x,y) \\ s_4(x,y) \end{pmatrix}, \tag{63}$$

$$\Psi \equiv \begin{pmatrix} \psi_1(x,y) \\ \psi_2(x,y) \\ \psi_3(x,y) \\ \psi_4(x,y) \end{pmatrix}. \tag{64}$$

Then Eq. (58) can be written

$$D\Psi + \Sigma\Psi = K\Psi + S. \tag{65}$$

Now assume that

$$\Psi^* \equiv \begin{pmatrix} \psi_1^*(x,y) \\ \psi_2^*(x,y) \\ \psi_3^*(x,y) \\ \psi_4^*(x,y) \end{pmatrix}.$$

is a solution of the adjoint system of equations:

$$(-D + \Sigma - K')\Psi^* = S^*(x,y)$$

where

$$0 < x < a, \quad 0 < y < b$$
$$\psi_1^*(a,y) = Q_1^*(y), \quad \psi_2^*(0,y) = Q_2^*(y),$$
$$\psi_3^*(x,b) = Q_3^*(x), \quad \psi_4^*(x,0) = Q_4^*(y).$$

Here K' is the matrix transpose of K and the functions

$$S^*(x,y) \equiv \begin{pmatrix} s_1^*(x,y) \\ s_2^*(x,y) \\ s_3^*(x,y) \\ s_4^*(x,y) \end{pmatrix} \tag{66}$$

are specified by the problem we wish to solve. That is, the problem is to estimate the inner product

$$I = (S^*, \Psi) = \begin{pmatrix} \int\int s_1^*(x,y)\psi_1(x,y)\mathrm{d}x\mathrm{d}y \\ +\int\int s_2^*(x,y)\psi_2(x,y)\mathrm{d}x\mathrm{d}y \\ +\int\int s_3^*(x,y)\psi_3(x,y)\mathrm{d}x\mathrm{d}y \\ +\int\int s_4^*(x,y)\psi_4(x,y)\mathrm{d}x\mathrm{d}y \end{pmatrix}.$$

Reciprocity then allows the conclusion (assuming that the boundary conditions for the adjoint system are dual to those for the original system, so that all boundary integrals vanish)

$$\begin{aligned}(S, \Psi^*) &= ((D+\Sigma-K)\Psi, \Psi^*) = (D\Psi, \Psi^*) + (\Sigma\Psi, \Upsilon^*) - (K\Psi, \Psi^*) = (\Psi, -D\Psi^*) + (\Psi, \Sigma\Psi^*) - (\Psi, K'\Psi^*) \\ &= (\Psi, (-D+\Sigma-K')\Psi^*) = (\Psi, S^*)\end{aligned}$$

Often it is more convenient to use the integral form of the RTE. If we assume that all the coefficient functions $\Sigma_t(x,y), \Sigma_s(x,y)$ do not depend on x or y, then Eq. (58) can be converted to the following system of integral equations:

$$\begin{cases} \psi_1(x,y) = \Sigma_s \sum_{j=1}^4 p_{1j} \int_0^x e^{-\sum_t (x-x')} \psi_j(x',y)\mathrm{d}x' + S_1(x,y), \\ \psi_2(x,y) = \sum_s \sum_{j=1}^4 p_{2j} \int_x^a e^{-\sum_t (x'-x)} \psi_j(x',y)\mathrm{d}x' + S_2(x,y), \\ \psi_3(x,y) = \sum_s \sum_{j=1}^4 p_{3j} \int_0^y e^{-\sum_t (y-y')} \psi_j(x,y')\mathrm{d}y' + S_3(x,y), \\ \psi_4(x,y) = \sum_s \sum_{j=1}^4 p_{4j} \int_y^b e^{-\sum_t (y'-y)} \psi_j(x,y')\mathrm{d}y' + S_4(x,y), \\ S_1(x,y) \equiv \int_0^x e^{-\sum_t (x-x')} s_1(x',y)\mathrm{d}x' + e^{-\sum_t x} Q_1(y), \\ S_2(x,y) \equiv \int_x^a e^{-\sum_t (x'-x)} s_2(x',y)\mathrm{d}x' + e^{-\sum_t (a-x)} Q_2(y), \\ S_3(x,y) \equiv \int_0^y e^{-\sum_t (y-y')} s_3(x,y')\mathrm{d}y' + e^{-\sum_t y} Q_3(x), \\ S_4(x,y) \equiv \int_y^b e^{-\sum_t (y'-y)} s_4(x,y')\mathrm{d}y' + e^{-\Sigma_t (b-y)} Q_4(x). \end{cases} \tag{67}$$

We write this in matrix form by defining the matrix K, where

$$\begin{aligned} K_{1j} &= \Sigma_s p_{1j} \int_0^x e^{-\Sigma_t (x-x')}\mathrm{d}x', \quad K_{3j} = \Sigma_s p_{3j} \int_0^y e^{-\Sigma_t (y-y')}\mathrm{d}y', \\ K_{2j} &= \Sigma_s p_{2j} \int_x^a e^{-\Sigma_t (x'-x)}\mathrm{d}x', \quad K_{4j} = \Sigma_s p_{4j} \int_y^b e^{-\Sigma_t (y'-y)}\mathrm{d}y' \end{aligned} \tag{68}$$

for $j = 1, \ldots, 4$. Then we have:

$$\Psi = K\Psi + S, \tag{69}$$

where

$$S \equiv \begin{pmatrix} S_1(x,y) \\ S_2(x,y) \\ S_3(x,y) \\ S_4(x,y) \end{pmatrix}. \tag{70}$$

Based on the algorithm described above, we have executed some tests for a wide range of choices of $\widehat{W}_0 =$ the number of random walks selected for each adaptive stage. As stated in the Remark following Theorem 4, the theory predicts very conservative values for W_0. However, much smaller values of W_0 can produce the sought geometric convergence. For instance, our numerical experiments show that $W_0 \cong 49,000$ produces stable geometric convergence for the data:

$$a = 5, \quad b = 4, \quad \sum_a = 0.5, \quad \sum_s = 0.5,$$

$$p_{ij} = \begin{pmatrix} 0.4 & 0.1 & 0.2 & 0.4 \\ 0.2 & 0.3 & 0.1 & 0.3 \\ 0.2 & 0.1 & 0.1 & 0.1 \\ 0.2 & 0.5 & 0.6 & 0.2 \end{pmatrix}$$

with boundary value functions (which concentrate the source on the $x = 0$ and $y = b$ boundary lines)

$$Q_1(y) = \frac{y}{b}, \quad 0 < y < b, \qquad Q_2(y) = 0, \quad 0 < y < b,$$

$$Q_3(x) = 0, \quad 0 < x < a, \quad Q_4(x) = 1 - \frac{x}{a}, \quad 0 < x < a.$$

For all of the numerical experiments reported here we represented the approximate solution as a 10th order polynomial in both x and y, so that $N = 100$ in Theorem 4. Fig. 1 plots the $\log_{10}$ values of the variances versus the number of adaptive stages for $W_0 = 50,000, 80,000$ and $100,000$ while Fig. 2 depicts the cases $W_0 = 60,000, 70,000, 80,000$ and 100,000 and concentrates attention on just the first 50 adaptive stages. We note that increasing W_0 does increase the rate of convergence, as the theory predicts, and results in a smaller number of stages to achieve a fixed precision. However, optimal *computational efficiency* requires a balance between the number of random walks per stage and the number of stages. If we ask, for example, which of the five choices of W_0 produces the most efficient computation, the answer may be found by fixing a desired level of accuracy, estimating the convergence rates from the slopes in the figures and calculating the run time required to achieve that for each choice of W_0. We can easily also estimate the computation time required to achieve any fixed error level with conventional Monte Carlo since the initial stage of each adaptive run is just conventional Monte Carlo based on W_0 random walks.

From Figs. 1 and 2, we can see that the first 50,000 random walks produces roughly 1.5 decimal digits of accuracy. Each additional decimal digit of accuracy will require roughly a 100-fold increase in the number of random walks based on the central limit theorem rate of convergence for conventional Monte Carlo. Since 50,000 random walks took about 404 s, to achieve an additional (say) 5 decimal digits of accuracy would require about 404×100^5 s, which is more than 1 year!

To illustrate how to estimate the run time to achieve this accuracy for each adaptive case, we select the case $W_0 = 60,000$. The run time per stage is about 485 s and the following table shows that this case produces a geometric error reduction factor of $\lambda = 0.747$. We next observe that the minimum stage number N to achieve reduction of the initial error by 5 additional decimal digits produces the inequality $\lambda^N \leqslant 10^{-5}$, establishing that $N = 40$ would suffice. We conclude that the total time needed for the case $W_0 = 60,000$ to achieve the same error reduction as in the conventional illustration would be $40 \times 485 = 19,400$ s, which is a little more than 5 h! The gain in computational efficiency resulting from the use of our algorithm compared with conventional Monte Carlo in this problem is thus $404 \times 100^5 / 40 \times 485 = 2.05 \times 10^7$.

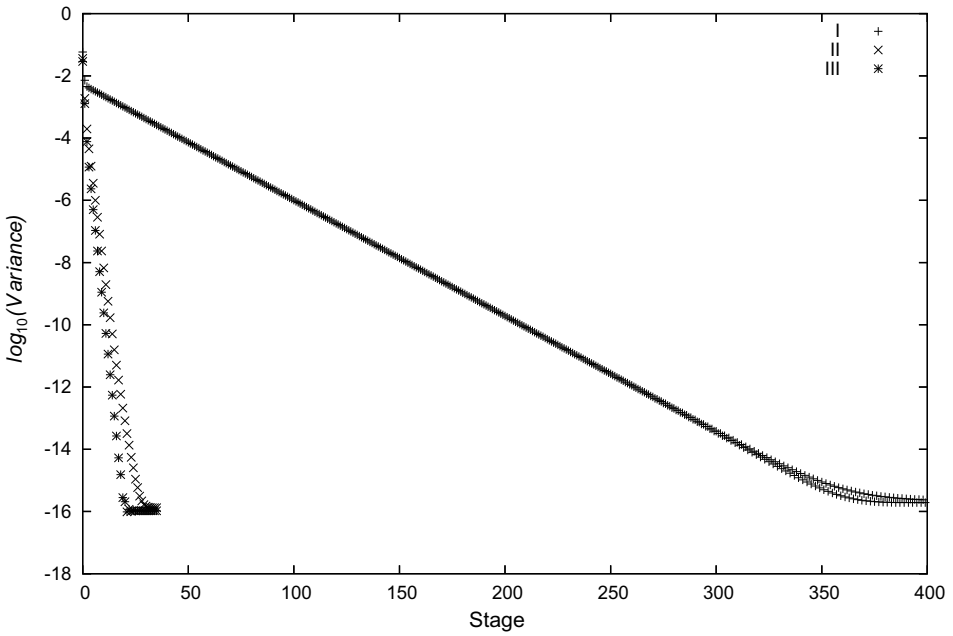

Fig. 1. Convergence characteristics for three choices of W_0; $I : W_0 = 50,000$; $II : W_0 = 80,000$; $III : W_0 = 100,000$.

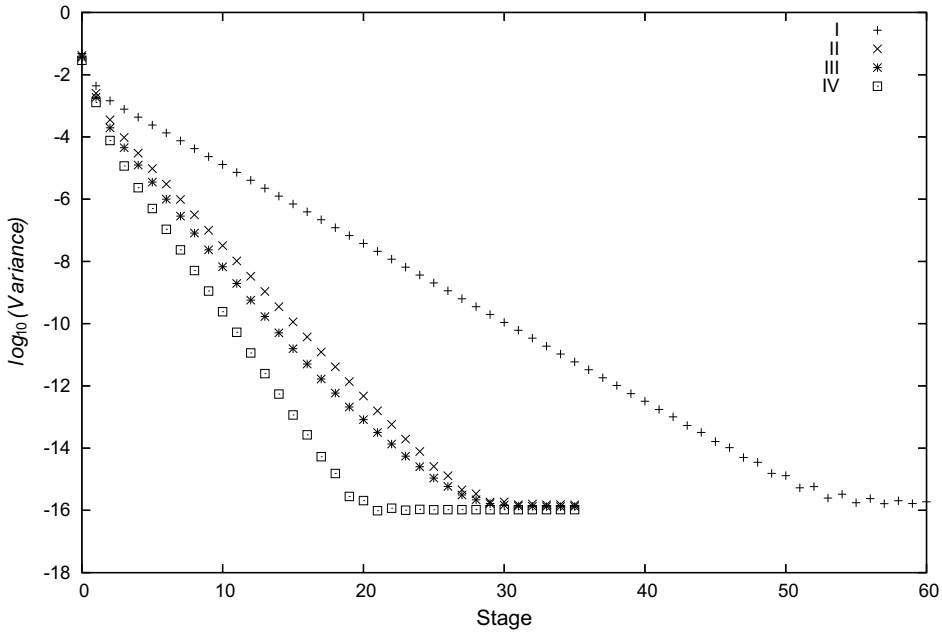

Fig. 2. Convergence characteristics for four choices of W_0; $I : W_0 = 60,000$; $II : W_0 = 70,000$; $III : W_0 = 80,000$; $IV : W_0 = 100,000$.

The following table displays the estimates of λ that correspond to the different values of W_0 for each of the 5 cases:

W_0	50,000	60,000	70,000	80,000	100,000
Estimated λ	0.958	0.747	0.57	0.549	0.465
Time per stage, in s	404	485	566	646	808

The table uses the inequality (1) to determine λ

$$E_m \leqslant \lambda E_{m-1},$$

where we have replaced the error term E_m by the standard deviation, since we do not have the exact solution for this problem. In summary, our analysis reveals that the case $W_0 = 70,000$ would require the least run time and is, therefore, the most efficient of the 5 chosen for this study.

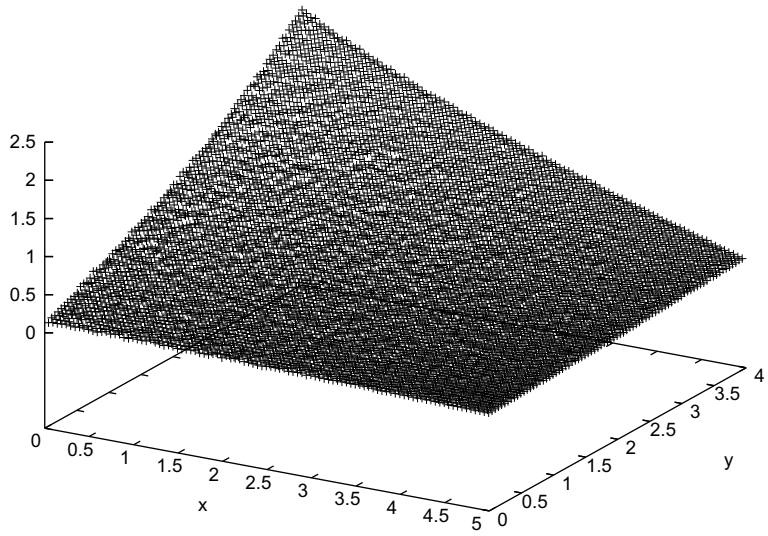

Fig. 3. Scalar flux for two dimensional transport problem.

Fig. 3 plots the scalar flux $\Psi(x,y)$ for this problem, which is simply the sum of the four component solutions since the angular dependence is discrete for this problem: $\Psi(x,y) = \sum_{i=1}^{4} \psi_i(x,y)$. Note especially the lack of any polynomial artifacts in this plot, even though the solution method represents the solution by a polynomial in each independent variable.

5. Summary, conclusions and future work

In this paper, we have constructed sequential Monte Carlo algorithms to solve a rather general family of transport problems and we have established rigorous conditions that will guarantee geometric convergence with probability 1. While our theory falls short of establishing both necessary and sufficient conditions for this accelerated convergence, numerical evidence strongly suggests that the sufficient conditions outlined here lead to quite conservative estimates of the number of random walks per stage that will assure geometric learning. The question then remains: how, in practice, one can determine adequate choices of W_0 that will assure geometric convergence without incurring large computational costs?

We have found that reliable error estimates can be based on the residual which, with the sequential correlated sampling method, is automatically computed at the end of each adaptive stage, since this function provides the source to the next adaptive stage. Our experience with this method is that it is very robust, producing very impressive results over a wide range of transport problems. As well, the residual and the error are closely coupled for many interesting applications (see, e.g. [15]). We are successfully applying the ideas of this paper to challenging practical problems for which a very accurate solution of the global transport equation is needed to serve as a computational "gold standard". Such methods are therefore playing a major role for a growing number of real problems for which either no other solution method is adequate, or as a standard against which to compare other less expensive and less accurate solution techniques.

In other publications we will provide similar results concerning the geometric convergence of adaptive Monte Carlo algorithms based on successive application of importance sampling estimators. Our conviction is that no single Monte Carlo method can hope to solve all transport problems equally well. Our experience, in fact, suggests that geometrically convergent importance sampling algorithms apply to some transport problems that are not as well treated by sequential correlated sampling algorithms as those described in this paper, and that both methods should be pursued.

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Appendix

Proof of Theorem 2

Remark. We rely on the following two basic formulas for the conditional mean and variance of any random variables X and Y,

$$E_X[X] = E_Y[E_X[X|Y]], \tag{A.1}$$

and

$$V_X[X] = E_Y[V_X[X|Y]] + V_Y[E_X[X|Y]]. \tag{A.2}$$

For proofs of these results, see [16].

Proof of Theorem 2. By conditioning on η_{P_0} and using (A.2), we obtain

$$V_\omega[\omega(P_0)] = E_\eta[V_\omega[\omega(P_0)|\eta_{P_0}]] + V_\eta[E_\omega[\omega(P_0)|\eta_{P_0}]], \tag{A.3}$$

where, and hereafter, $V_\omega \equiv V_{\omega(\cdot)}$, $E_\omega \equiv E_{\omega(\cdot)}$, $V_\eta \equiv V_{\eta_P}$, $E_\eta \equiv E_{\eta_P}$, and so on. We have

$$V_\omega[\omega(P_0)] = V_\omega[\omega(P_0)|\eta_{P_0} = 1]\hat{p}(P_0) + V_\omega[\omega(P_0)|\eta_{P_0} = 0](1-\hat{p}(P_0)) + E_\eta[E_\omega[\omega(P_0)|\eta_{P_0}]]^2 - \{E_\eta[E_\omega[\omega(P_0)|\eta_{P_0}]]\}^2. \tag{A.4}$$

The first term of the right hand side is equal to zero because, under the condition $\eta_{P_0} = 1$, $\omega(P_0)$ is deterministic, while the last term is equal to $(E_\omega[\omega(P_0)])^2$, owing to (A.1). Again, applying (A.1) on the second term by conditioning $(.\omega(P_0)|\eta_{P_0} = 0)$ on ξ_1, we obtain

$$\begin{aligned} V_\omega[\omega(P_0)] &= E_\xi[V_\omega[\omega(P_0)|\eta_{P_0} = 0, \xi_1]](1-\hat{p}(P_0)) + V_\xi[E_\omega[\omega(P_0)|\eta_{P_0} = 0, \xi_1]](1-\hat{p}(P_0)) + [E_\omega[\omega(P_0)|\eta_{P_0} \\ &= 1]]^2\hat{p}(P_0) + [E_\omega[\omega(P_0)|\eta_{P_0} = 0]]^2(1-\hat{p}(P_0)) - (E_\omega[\omega(P_0)])^2 = \int_\Gamma V_\omega[\omega(P_0)|\eta_{P_0} = 0, \xi_1 \\ &= Q]\widehat{K}(P_0, Q)\mathrm{d}Q + E_\xi[E_\omega[\omega(P_0)|\eta_{P_0} = 0, \xi_1]]^2(1-\hat{p}(P_0)) - \{E_\xi[E_\omega[\omega(P_0)|\eta_{P_0} \\ &= 0, \xi_1]]\}^2(1-\hat{p}(P_0)) + (S(P_0))^2\hat{p}(P_0) + [E_\omega[\omega(P_0)|\eta_{P_0} = 0]]^2(1-\hat{p}(P_0)) - (E_\omega[\omega(P_0)])^2, \end{aligned} \tag{A.5}$$

where, it can be easily verified that $E_\omega[.\omega(P_0)|\eta_{P_0}=1]=S(P_0)$. According to (A.1), the third term and the fifth term cancel out. We then have

$$V_\omega[\omega(P_0)]=\int_\Gamma V_\omega[\omega(P_0)|\eta_{P_0}=0,\xi_1=Q]\widehat{K}(P_0,Q)\mathrm{d}Q+\int_\Gamma\{E_\omega[\omega(P_0)|\eta_{P_0}=0,\xi_1=Q]\}^2\widehat{K}(P_0,Q)\mathrm{d}Q+(S(P_0))^2\hat{p}(P_0)-(E_\omega[\omega(P_0)])^2. \tag{A.6}$$

According to the definition of $\omega(P_0)$, (11), we have

$$(\omega(P_0)|\eta_{P_0}=0,\xi_1=Q)=S(P_0)+\frac{K(P_0,Q)}{\widehat{K}(P_0,Q)}\omega(Q). \tag{A.7}$$

Substituting this into (A.6) produces

$$V_\omega[\omega(P_0)]=\int_\Gamma V_\omega[S(P_0)+\frac{K(P_0,Q)}{\widehat{K}(P_0,Q)}\omega(Q)]\widehat{K}(P_0,Q)\mathrm{d}Q+\int_\Gamma\left\{E_\omega[S(P_0)+\frac{K(P_0,Q)}{\widehat{K}(P_0,Q)}\omega(Q)]\right\}^2\widehat{K}(P_0,Q)\mathrm{d}Q+(S(P_0))^2\hat{p}(P_0)-(E_\omega[\omega(P_0)])^2. \tag{A.8}$$

Using (12), we finally obtain an equation governing $V_\omega[\omega(P_0)]$

$$V_\omega[\omega(P_0)]=\int_\Gamma\left(\frac{K(P_0,Q)}{\widehat{K}(P_0,Q)}\right)^2V_\omega[\omega(Q)]\widehat{K}(P_0,Q)\mathrm{d}Q+\int_\Gamma(S(P_0)+\frac{K(P_0,Q)}{\widehat{K}(P_0,Q)}\omega(Q))^2\widehat{K}(P_0,Q)\mathrm{d}Q+(S(P_0))^2\hat{p}(P_0)-(\Psi(P_0))^2, \tag{A.9}$$

or

$$V_\omega[\omega(P_0)]+(\Psi(P_0))^2=\int_\Gamma\left(\frac{K(P_0,Q)}{\widehat{K}(P_0,Q)}\right)^2(V_\omega[\omega(Q)]+(\Psi(Q))^2)\widehat{K}(P_0,Q)\mathrm{d}Q+(S(P_0))^2+2S(P_0)\int_\Gamma K(P_0,Q)\Psi(Q)\mathrm{d}Q. \tag{A.10}$$

Since $\int_\Gamma K(P_0,Q)\Psi(Q)\mathrm{d}Q=\Psi(P_0)-S(P_0)$, we have

$$V_\omega[\omega(P_0)]+(\Psi(P_0))^2=\int_\Gamma\left(\frac{K(P_0,Q)}{\widehat{K}(P_0,Q)}\right)^2\left(V_\omega[\omega(Q)]+(\Psi(Q))^2\right)\widehat{K}(P_0,Q)\mathrm{d}Q+(\Psi(P_0))^2-(\Psi(P_0)-S(P_0))^2. \tag{A.11}$$

(14) is proved. Now, let us prove (15). Applying (A.2)–(A.10), we obtain

$$V_\zeta[\zeta]=E_\xi[V_\zeta[\zeta|\xi_0]]+V_\xi[E_\zeta[\zeta|\xi_0]]=\int_\Gamma V_\zeta[\zeta|\xi_0=P]\widehat{S}(P)\mathrm{d}P+E_\xi[E_\zeta[\zeta|\xi_0]]^2-\{E_\xi[E_\zeta[\zeta|\xi P_0]]\}^2$$
$$=\int_\Gamma V_\zeta\left[\frac{S^*(P)}{\widehat{S}(P)}\omega(P)\right]\widehat{S}(P)\mathrm{d}P+\int_\Gamma\left\{E_\zeta\left[\frac{S^*(P)}{\widehat{S}(P)}\omega(P)\right]\right\}^2\widehat{S}(P)\mathrm{d}P-\{E_\xi[E_\zeta[\zeta|\xi_0]]\}^2. \tag{A.12}$$

Using (A.2) and (A.10), we finally obtain a formula for $V_\zeta[\zeta]$

$$V_\zeta[\zeta]=\int_\Gamma\left(\frac{S^*(P)}{\widehat{S}(P)}\right)^2V_\omega[\omega(P)]\widehat{S}(P)\mathrm{d}P+\int_\Gamma\left(\frac{S^*(P)}{\widehat{S}(P)}\right)^2(\Psi(P))^2\widehat{S}(P)\mathrm{d}P-\langle\Psi,S^*\rangle^2, \tag{A.13}$$

or

$$V_\zeta[\zeta]+\langle\Psi,S^*\rangle^2=\int_\Gamma\left(\frac{S^*(P)}{\widehat{S}(P)}\right)^2(V_\omega[\omega(P)]+(\Psi(P))^2)\widehat{S}(P)\mathrm{d}P. \tag{A.14}$$

The proof is completed. □

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