LA-UR- 97-2402

Title: EXPONENTIAL CONVERGENCE WITH ADAPTIVE MONTE CARLO

CONF-971125--

Author(s): Thomas E. Booth

Submitted to: American Nuclear Society 1997 Winter Meeting, November 16-20, 1997, Albuquerque, NM

Los Alamos
NATIONAL LABORATORY

DISCLAIMER

EXPONENTIAL CONVERGENCE WITH ADAPTIVE MONTE CARLO

T. E. Booth

Los Alamos National Laboratory

I. INTRODUCTION

For over a decade, it has been known that exponential convergence on discrete transport problems was possible using adaptive Monte Carlo techniques. Now, exponential convergence has been empirically demonstrated on a spatially continuous problem.

II. THE SPATIALLY CONTINUOUS BIDIRECTIONAL TRANSPORT PROBLEM

The test problem transports particles on a line of length T; that is, $0 \leq x \leq T$. The particles can move either forward ($\mu = 1$) or backward ($\mu = -1$) on the line. The particles are sourced in moving forward at x=0. The particles score $1 + \delta$ if they escape at $x = T$ and δ otherwise. That is, δ plus the penetration probability is being estimated.

III. ZERO VARIANCE BIASING

Zero variance biasing can be done on any linear Monte Carlo calculation,[1] whether the calculation is analog or uses any arbitrary variance reduction techniques, such as splitting or forced collisions. Zero variance biasing occurs when *every* event is sampled proportional to its natural probability times the expected score thereafter produced if the event were to be sampled. That is, the sampling is importance weighted.

The expected score, or *importance*, is a function of position and direction. The six definitions below are necessary to derive the importance equations.

Definition 1. $N(x)$ = the expected score from a particle moving forward at x.

Definition 2. $L(x)$ = the expected score from a particle moving backward at x.

Definition 3. f = probability of scattering forward (i.e., no change in direction).

Definition 4. r = probability of scattering backward (i.e., a direction reversal on scattering).

Definition 5. σ = the total cross section.

Definition 6. σ_s = the scattering cross section.

IV. IMPORTANCE FUNCTION EXPANSION AT A POINT

The differential equations for the importance can be obtained from standard textbooks[2] by putting in Dirac-δ functions for all variables except space. The result is

$$N'(x) = (\sigma - \sigma_s f)N(x) - \sigma_s r L(x) - [\sigma - \sigma_s]\delta \tag{1}$$

$$L'(x) = -(\sigma - \sigma_s f)L(x) + \sigma_s r N(x) + [\sigma - \sigma_s]\delta \tag{2}$$

Suppose one takes n more derivatives

$$N^{(n+1)}(x) = (\sigma - \sigma_s f)N^{(n)}(x) - \sigma_s r L^{(n)}(x) \tag{3}$$

$$L^{(n+1)}(x) = -(\sigma - \sigma_s f)L^{(n)}(x) + \sigma_s r N^{(n)}(x) \tag{4}$$

Note that if at some particular point y both $N(y)$ and $L(y)$ are known, then *all* derivatives are known at y through equations 1-4. This suggests writing the importance function as the Taylor series

$$N(x) = \sum_{i=0}^{\infty} N^{(i)}(x)\Big|_{x=y} \frac{(x-y)^i}{i!} \tag{5}$$

$$L(x) = \sum_{i=0}^{\infty} L^{(i)}(x)\Big|_{x=y} \frac{(x-y)^i}{i!} \tag{6}$$

(Note that Eqs. 3 and 4 assume a constant medium, but as long as σ, σ_s, r, and f are analytic, then one can obtain all derivatives of Eqs. 1 and 2 and do a Taylor expansion.)

A code was written to estimate $N(y)$ and $L(y)$ (with $y = T/2$) and then obtain the Taylor expansions of Eqs. 5 and 6. All samplings were then zero variance biased using the estimated importance function. Figure 1 shows exponential convergence on a one mean free path problem using a Taylor series of order 50 and 1000 particles per iteration. This is the first example of exponential convergence on a continuous transport problem.

V. FALSE CONVERGENCE

It is worth noting that sometimes the importance weighted sampling converged exponentially fast to the *wrong* answer. This occurred when the derivative of the importance function became too large. The derivatives can be bounded using Eqs. 1 and 2:

$$N'(x) \leq (\sigma - \sigma_s f)N(x) - [\sigma - \sigma_s]\delta \tag{7}$$

$$-L'(x) \leq (\sigma - \sigma_s f)L(x) - [\sigma - \sigma_s]\delta \tag{8}$$

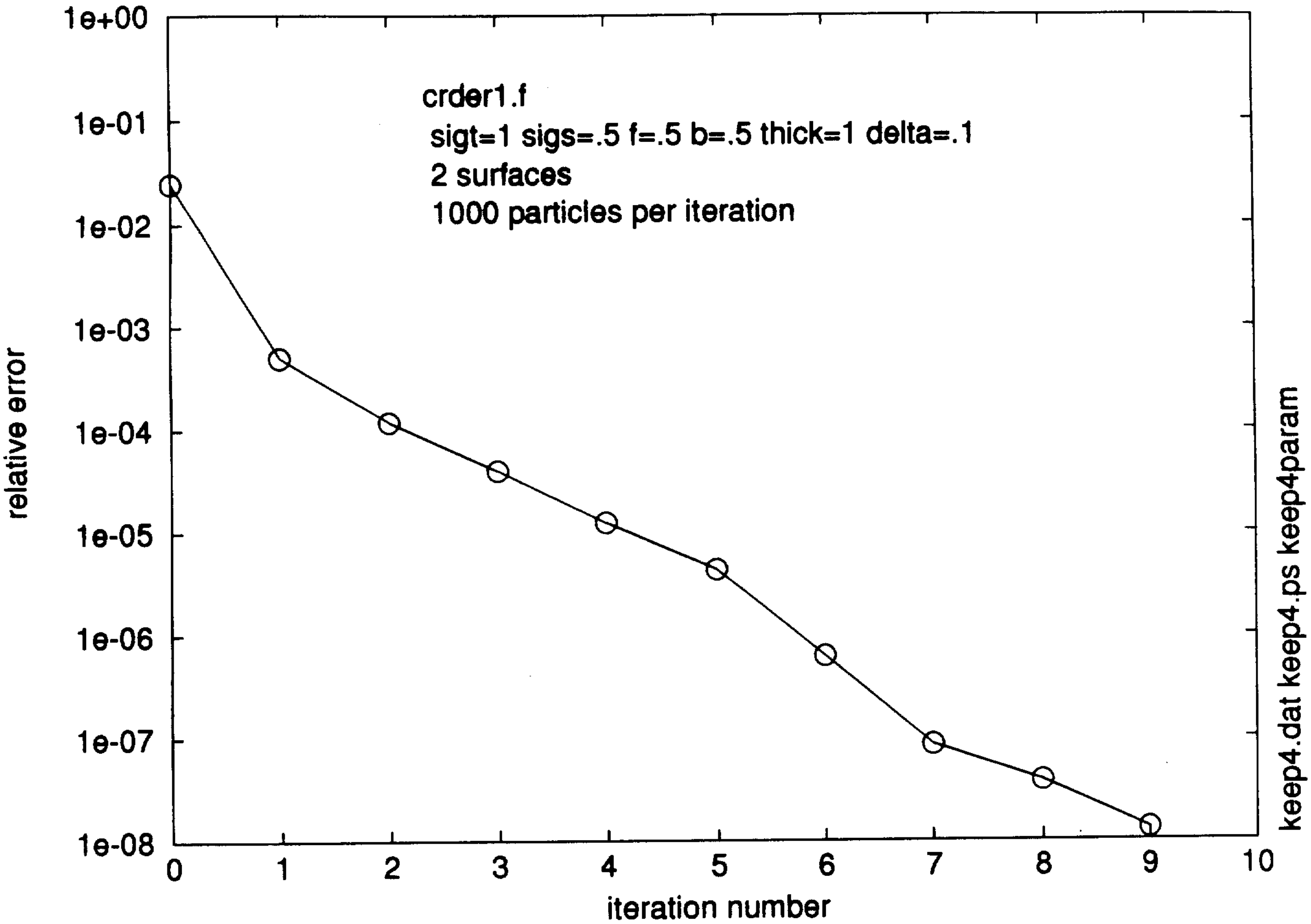

Fig. 1. Exponential Convergence by Taylor Expansion.

If these bounds were violated, then the zero-th term of the corresponding Taylor series was increased enough to satisfy these bounds (for all x), while keeping all other terms constant. This seems to prevent false convergence.

VI. CONCLUSION AND FUTURE WORK

Exponential convergence was obtained on a spatially continuous transport problem by embedding the importance equation into the Monte Carlo estimation of the importance function. Although not discussed here, several direct attempts at estimating the importance function *without* embedding the importance equation failed to produce exponential convergence. This hints that exponential convergence for more complicated transport problems probably also will require embedding the importance equation into the importance estimation procedure. Exponential convergence for the one-speed slab problem is currently being studied.

REFERENCES

1. T. E. Booth, *Nucl. Sci. Eng.,* **102**, 332 (1989).
2. G. I. Bell and S. Glasstone, "Nuclear Reactor Theory," 1970, Litton Educational Publishing, Inc., pages 262-263.

M97009130

Report Number (14) LA-UR--97-2402
CONF-971125--

Publ. Date (11) 199708
Sponsor Code (18) DOE/MA, XF
UC Category (19) UC-910, DOE/ER

DOE