LA-UR-01-0675
Approved for public release;
distribution is unlimited.

Title:

Monte Carlo Particle Transport in Media with Exponentially Varying Time-dependent Cross-sections

Author(s):

Forrest B. Brown & William R. Martin

Submitted to:

http://lib-www.lanl.gov/la-pubs/00367066.pdf

Monte Carlo Particle Transport in Media with Exponentially Varying Time-dependent Cross-sections

Forrest B. Brown & William R. Martin

X-3 Group, Applied Physics Division
Los Alamos National Laboratory
Los Alamos, NM 87545
<fbrown@lanl.gov>

Introduction

We have investigated Monte Carlo schemes for analyzing particle transport through media with exponentially varying time-dependent cross-sections. For such media, the cross-sections are represented in the form

$$\Sigma(t) = \Sigma_0 \, \mathrm{e}^{-at} \tag{1}$$

or equivalently as

$$\Sigma(x) = \Sigma_0 \, \mathrm{e}^{-bx} \tag{2}$$

where b=av and v is the particle speed. For the discussion below, the parameters a and b may be either positive, for exponentially decreasing cross-sections, or negative, for exponentially increasing cross-sections. For most time-dependent Monte Carlo applications, the time and spatial variation of the cross-section data are handled by means of a stepwise procedure, holding the cross-sections constant for each region over a small time interval Δt, performing the Monte Carlo random walk over the interval Δt, updating the cross-sections, and then repeating for a series of time intervals. Continuously varying spatial- or time-dependent cross-sections can be treated in a rigorous Monte Carlo fashion using delta-tracking [1], but inefficiencies may arise if the range of cross-section variation is large. In this summary, we present a new method for sampling collision distances directly for cross-sections which vary exponentially in space or time. The method is exact and efficient, and has direct application to Monte Carlo radiation transport methods.

Derivation of the PDF for collision distance

The Monte Carlo procedure of interest is the random sampling of a distance-to-collision, given that the region interaction cross-section varies as in Eq. (1) or (2). Other operations such as pathlength or collision tallies are relatively straightforward. For convenience, we will assume the cross-section behavior given by Eq. (2), with exponential variation along a flight path. For a particle starting a free-flight from position x=0, the probability of not colliding in a distance x is given by

$$P_{NC}(x) \;=\; \exp\left(-\int_0^x \Sigma(x')dx' \right) \;=\; \exp\left(-\frac{\Sigma_0}{b}(1-e^{-bx}) \right) \tag{3}$$

In the limit of $b \rightarrow 0$, Eq. (3) reduces to the standard transmission probability for constant cross-section, $\exp(-\Sigma_0 x)$. Defining P_C to be the probability of colliding in a finite distance of travel,

$$P_C \;=\; 1 - P_{NC}(\infty) \;=\; \begin{cases} 1 - e^{-\Sigma_0 / b} & \text{for } b > 0, \\ 1 & \text{for } b \le 0 \end{cases} \tag{4}$$

Then, the probability density function (PDF) for the collision distance s may be given as

$$\begin{aligned} f(s) &= (1 - P_C)\cdot\delta(s=\infty) \;+\; P_C \cdot \Sigma(s) \cdot P_{NC}(s)/c \\ &= (1 - P_C)\cdot\delta(s=\infty) \;+\; P_C \cdot \Sigma(s) \cdot \exp\left(-\int_0^s \Sigma(x)dx\right)/c, \quad 0 \le s < \infty \end{aligned}$$

where (5)

$$c = \int_0^\infty \Sigma(s) \exp\left(-\int_0^s \Sigma(x)dx\right) ds$$

and $\delta = \text{Dirac delta function}$

The first term in Eq. (5) accounts for the possibility that the distance to collision may be infinite, that is, that no collision occurs in a finite distance. This can occur only for the case of an exponentially decreasing cross-section. The second term accounts for the possibility that a collision will occur after a free-flight of distance s. The constant c is simply the normalization factor for the collision probability and is determined below.

Let $$y = \int_0^s \Sigma(x)dx \;=\; \int_0^s \Sigma_0\, e^{-bx}\, dx \;=\; \frac{\Sigma_0}{b}(1 - e^{-bs}) \tag{6}$$

Note that the range of y is $(0, \Sigma_0 / b)$ for $b>0$, and $(0,\infty)$ for $b \le 0$.

Then,

$$\begin{aligned} c &= \int_0^\infty \Sigma(s) \exp\left(-\int_0^s \Sigma(x)dx\right) ds \\ &= \begin{cases} \displaystyle\int_0^{\Sigma_0/b} e^{-y}\, dy = 1 - e^{-\Sigma_0/b} & \text{for } b > 0, \\ \displaystyle\int_0^\infty e^{-y}\, dy = 1 & \text{for } b \le 0. \end{cases} \end{aligned} \tag{7}$$

Random Sampling Procedure

During Monte Carlo calculations, it is necessary to randomly sample the distance to collision from the PDF given by Eq. (5), that is, to solve the following equation for $\hat{s}$:

$$\xi \;=\; \int_0^{\hat{s}} f(s)ds, \qquad \text{where } \xi \text{ is a random number in } (0,1) \tag{8}$$

This may be done in a straightforward manner, using standard techniques for first discrete sampling to select whether or not a collision occurs, and then (if one did) to sample from either an exponential or a truncated exponential probability density [2]. The procedure is:

For $b<0$:

$$f(y) = f(s)\frac{ds}{dy} = e^{-y}, \qquad 0 \le y < \infty$$

which can be sampled by $\hat{y} = -\ln(\xi)$

(9)

Then, Eq. (6) can be used to solve for $\hat{s}$:

$$\hat{s} \;=\; -\tfrac{1}{b}\cdot \ln(1-\tfrac{b}{\Sigma_0}\hat{y})$$

For $b=0$,

$$\hat{s} = -\tfrac{1}{\Sigma_0}\ln(\xi) \tag{10}$$

For $b>0$,

$$f(s) = (1-P_C)\cdot\delta(s=\infty) + P_C\cdot\frac{e^{-y}}{1-e^{-\Sigma_0/b}}, \qquad 0 \le y \le (\Sigma_0/b)$$

which can be sampled by:

if $\xi_1 > P_C$, $\hat{s} = \infty$ (11)

else

$\hat{y} = -\ln[1-\xi_2\cdot(1-e^{-\Sigma_0/b})]$

and using Eq. (6),

$\hat{s} = -\tfrac{1}{b}\cdot\ln(1-\tfrac{b}{\Sigma_0}\hat{y})$

Numerical Results

To verify that the PDF given by Eq. (5) is correct and that the random sampling procedure yields correct results, numerical experiments were performed using a 1-D Monte Carlo code. The physical problem consisted of a beam source impinging on a purely absorbing infinite slab, with a slab thickness of 1 cm and $\Sigma_0 = 1\ \mathrm{cm}^{-1}$. Monte Carlo calculations with 10,000 particles were run for a range of the exponential parameter *b* from $-5\ \mathrm{cm}^{-1}$ to $+20\ \mathrm{cm}^{-1}$. Two separate Monte Carlo calculations were run for each choice of *b*, a continuously varying case using the random sampling procedures described above, and a “conventional” case where the exponential variation in cross-section was described in a stepwise approximation using 250 separate regions of constant cross-section. For each calculation, transmission through the outer boundary of the slab was tallied. The results shown in Figure (1) show nearly perfect agreement in transmission over the range of exponential parameters for the varying cross-section, verifying that the PDF and random sampling procedure described above are correct.

Conclusions

A PDF and random sampling procedure for the distance to collision were derived for the case of exponentially varying cross-sections. Numerical testing indicates that both are correct. This new sampling procedure has direct application in a new method for Monte Carlo radiation transport [3], and may be generally useful for analyzing physical problems where the material cross-sections change very rapidly in an exponential manner.

References

1. L. L. Carter, E. D. Cashwell, & W. M. Taylor, “Monte Carlo Sampling with Continuously Varying Cross Sections Along Flight Paths”, *Nucl. Sci. Eng.* **48**, 403-411 (1972).

2. C. J. Everett & E. D. Cashwell, “A Third Monte Carlo Sampler”, Los Alamos National Laboratory report, LA-9721-MS (March, 1983).

3. W. R. Martin & F. B. Brown, “The Analytical Monte Carlo Method for Radiation Transport Calculations”, *Trans. Am. Nucl. Soc.* [submitted for this meeting], (2001).

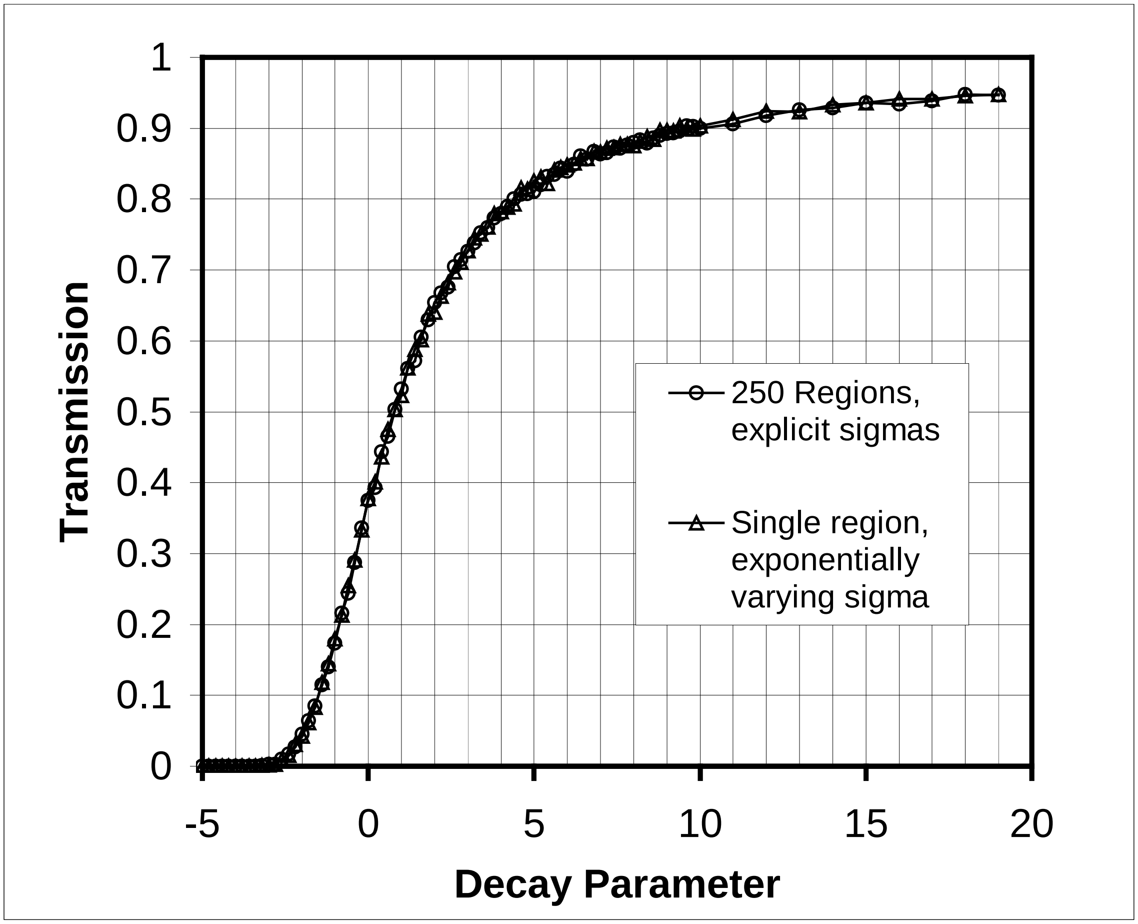

Figure 1. Transmission through a 1 mfp thick infinite slab as a function of cross-section decay parameter. Direct sampling from continuously varying cross-section compared with 250 regionwise cross-sections.