Woodcock tracking with arbitrary sampling cross section using negative weights

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ABSTRACT:

The paper presents a variant of the Woodcock free flight distance sampling algorithm. Instead of the majorant cross section of the whole system, an arbitrarily chosen cross section can be used for sampling the free flight distance. The novel algorithm may cause particle weights to become negative. This technique circumvents the major drawback of conventional Woodcock sampling when a localized heavy absorber implies much more frequent path sampling than required thereby rendering the calculation ineffective. Theoretical derivation is shown for heterogeneous medium. A one dimensional analytical and numerical model is presented for basic optimisation study of the free sampling parameters and an applied case illustration is shown using a GPU-based radiotherapy Monte Carlo code.

HIGHLIGHTS

- unbiased Woodcock tracking methodology using arbitrary sampling cross section
- one dimensional test case with analytical variance, runtime and efficiency formulas for better understanding the free sampling parameters
- illustration with 3D radiotherapy problem with efficiency gain of a factor 200

1 Introduction

Since its invention, Woodcock (delta-) tracking for particle transport free flight sampling [1] remained an integral part of the Monte Carlo (MC) knowledge base, routinely discussed in textbooks of the field [2,3]. Woodcock tracking has been implemented in many codes of the nuclear field for shielding (e.g. McBend, [4]), medical (e.g. [5]) and reactor applications (e.g. Serpent, [6]), moreover it has found its way to the Computer Graphics (CG) field ([7,8]). Instead of the Woodcock method, the most popular choice for free flight sampling is the surface to surface tracking of particles, and we will refer to this as 'ray marching' in this paper, a term borrowed from the CG field. The major drawback associated with Woodcock tracking is the adverse effect of a localized heavy absorber on computation efficiency quoted almost in every publication of the topic [e.g. 7,9,10]. In this paper we explore a modified Woodcock sampling scheme that does not require choosing the majorant cross section for the path length sampling but an arbitrary cross section may be used without introducing any bias of the probability density function. The scheme would result in some particle weight becoming negative. We emphasize that this method is not proposed as a standalone variance reduction technique, but rather as a building block of a more complex variance reduction scheme.

This paper is organized as follows: first we show the derivation of the modified sampling with a special introduction to using negative weights. Next, we show a 1D optimisation framework for transmission estimation with closed analytical expressions for the variance, estimated computer time and efficiency in terms of Figure of Merit (FoM). In order to indicate the applicability of the method under real word conditions a dedicated, GPU (Graphics Processing Unit) based radiotherapy code has been modified to include the new sampling technique and considerable gain in FoM is shown.

2 Theory

2.1 A short introduction to using negative weights at transport sampling

It is rather uncommon to use negative weights at nuclear MC transport calculations though not unprecedented [11, 12] therefore we dedicate a small section for their interpretation. There is a reason to the infrequent application: if we interpret a MC calculation as a simulation that mimics nature as closely as possible, the particle weight equals one, and can be thought of as a single particle, a modification to this scheme challenges intuition. Particle weights between 0 and 1 may be interpreted as a fraction of a bundle of particles. We propose that negative weights may be paraphrased as a compensation for another probability law that delivered more particles than it should have compared to the original physical law.

Let us model the MC estimation as an integral of a probability density function $f(P)$ multiplied by a detector function $D(P)$ and the product integrated over the whole phase space domain (Γ):

$$R = \int_{\Gamma} f\left(P\right) D\left(P\right) dP \tag{2.1}$$

with P standing for a set of phase space coordinates like position, solid angle, energy, time, or in an even more general way $P=(P_{n,1},\dots P_{n,m})$ could stand for the set of phase space coordinates of the n^{th} progeny from source event to an m^{th} collision. At the MC calculation, samples are drawn from $f(P)$ resulting in a phase space coordinate P_i and a weight w_i. The estimates are averages of the contributions $c_i = D(P_i)w_i$ over every history.

We can forge negative contributions by choosing D as a negative valued function, e.g. using Legendre polynomials for scoring [13], or just if we calculate the net current flowing outward of a surface where particles flying backwards count as negative. For a simple, though rather artificial example we can express $f(P) = g(P) - h(P)$ with g and h both pdf's, use a random number to decide with equal chances which of the two functions are sampled, and if h is selected then particle weight starts as negative.

2.2 Woodcock sampling with negative weights

The basic idea of standard Woodcock tracking is that instead of sampling the local cross section we can use an arbitrary cross section for sampling as long as that cross section is larger than any other in the system. A collision point is rejected if a random number does not check against the ratio of the sampling cross section and the true cross section of a location, in this case again a free path is selected using the sampling cross section and the particle flies on until the next sampled collision point candidate. The advantage lies in the freedom that free flight tracking would not be evaluated through every cell boundary crossing but only at positions of collision point candidates.

Let us review first the theory behind Woodcock sampling for a homogenous medium. The reason to this simplification is didactical, we give the full derivation for inhomogeneous medium in the Appendix. Let the actual sampling take place in a medium with Σ cross section, while the whole system majorant cross section is denoted by Σ_{maj}; thus $\Sigma < \Sigma_{maj}$. First we select a free path sample x_1 from $\Sigma_{maj}\, exp(-\Sigma_{maj}\, x)$ and accept it with probability Σ/Σ_{maj} by checking it against a canonically distributed random number. If the acceptance draw has failed (with probability $1-\Sigma/\Sigma_{maj}$), a virtual (delta) scatter has occurred and the particle proceeds without change of direction or energy, thus we sample $\Sigma_{maj}\, exp(-\Sigma_{maj}\, x)$ again to yield x_2, and accept it with probability Σ/Σ_{maj}. The pdf of the random variable x_1+x_2 is the convolution $\Sigma_{maj}\, exp(-\Sigma_{maj}\, x) * \Sigma_{maj}\, exp(-\Sigma_{maj}\, x)$ that it is analytically calculable, moreover any further chain convolutions are. Following this logic we can calculate the pdf of the above algorithm:

$$
\begin{aligned}
&\frac{\Sigma}{\Sigma_{maj}}\Sigma_{maj}e^{-\Sigma_{maj}x}+\left(1-\frac{\Sigma}{\Sigma_{maj}}\right)\frac{\Sigma}{\Sigma_{maj}}\Sigma_{maj}e^{-\Sigma_{maj}x}*\Sigma_{maj}e^{-\Sigma_{maj}x}+\\
&+\left(1-\frac{\Sigma}{\Sigma_{maj}}\right)^2\frac{\Sigma}{\Sigma_{maj}}\Sigma_{maj}e^{-\Sigma_{maj}x}*\Sigma_{maj}e^{-\Sigma_{maj}x}*\Sigma_{maj}e^{-\Sigma_{maj}x}+\ldots=\\
&=\frac{\Sigma}{\Sigma_{maj}}\Sigma_{maj}e^{-\Sigma_{maj}x}+\left(1-\frac{\Sigma}{\Sigma_{maj}}\right)\frac{\Sigma}{\Sigma_{maj}}x\Sigma_{maj}{}^2e^{-\Sigma_{maj}x}+\left(1-\frac{\Sigma}{\Sigma_{maj}}\right)^2\frac{\Sigma}{\Sigma_{maj}}\Sigma_{maj}{}^3\frac{x^2}{2}e^{-\Sigma_{maj}x}+\\
&\ldots+\left(1-\frac{\Sigma}{\Sigma_{maj}}\right)^{n-1}\frac{\Sigma}{\Sigma_{maj}}\Sigma_{maj}{}^n\frac{x^{n-1}}{(n-1)!}e^{-\Sigma_{maj}x}=\\
&=\sum_{n=1}^{\infty}\Sigma\frac{\left(\Sigma_{maj}-\Sigma\right)^{n-1}x^{n-1}}{(n-1)!}e^{-\Sigma_{maj}x}=\Sigma e^{\Sigma_{maj}x-\Sigma x-\Sigma_{maj}x}=\Sigma e^{-\Sigma x}
\end{aligned}
\tag{2.2}
$$

The derivation shows that the resulting sampling is equivalent to sampling *Σ exp(-Σ x)*. If we would like to choose $\Sigma > \Sigma_{maj}$, a hit would have probability above 1 and a miss would have negative probability, in other words we would never reject a collision candidate but would still get a biased estimate as only the first term of Eq.(2.2) would be sampled and the rest would be left out for good. We should notice that the expansion still holds regardless of the choice of the sampling cross section, therefore we can devise a different sampling scheme to obtain adequate samples for every term.

Let us choose an arbitrary sampling probability $0<q<1$, choose Σ_{samp} cross section for the path sampling, and introduce them into the series without altering the result:

$$
\begin{aligned}
\Sigma e^{-\Sigma x}&=\frac{\Sigma}{\Sigma_{maj}}\frac{1}{q}q\Sigma_{maj}e^{-\Sigma_{maj}x}+\left(\frac{1-\frac{\Sigma}{\Sigma_{maj}}}{1-q}\right)(1-q)\frac{\Sigma}{\Sigma_{samp}}\frac{1}{q}qx\Sigma_{samp}{}^2e^{-\Sigma_{samp}x}+\ldots\\
&\ldots+\left(\frac{1-\frac{\Sigma}{\Sigma_{samp}}}{1-q}\right)^{n-1}(1-q)^{n-1}\frac{\Sigma}{\Sigma_{samp}}\frac{1}{q}q\Sigma_{samp}{}^n\frac{x^{n-1}}{(n-1)!}e^{-\Sigma_{samp}x}
\end{aligned}
\tag{2.3}
$$

Let us now use q for collision acceptance probability and in case of a hit, let us compensate for this by multiplying the particle weight by $\Sigma/(q\Sigma_{samp})$ and accept the sample from sampling $\Sigma_{samp}\, exp(-\Sigma_{samp}\, x)$. In case of a miss (with probability $1-q$) let us multiply the particle weight by

$$
\left(\frac{1-\frac{\Sigma}{\Sigma_{samp}}}{1-q}\right) \tag{2.4}
$$

and carry on with the same procedure by selecting again a further flight path from Σ_{samp} $\exp(-\Sigma_{samp}\ x)$. In this way the infinite series are properly sampled and the Σ_{samp} sampling cross section is not restricted to the majorant.

If we choose $q = \Sigma/(\Sigma_{maj})$ and $\Sigma_{samp} = \Sigma_{maj}$, Eq.(2.4) yields a weight multiplier of 1 and we get the original Woodcock algorithm. If $\Sigma > \Sigma_{samp}$, the weight factor becomes negative if a virtual collision occurs.

The above sampling scheme yields an unbiased game also in an inhomogeneous system; the proof thereof is presented in the Appendix.

3 A one dimensional optimization scheme

We have analyzed a one dimensional test case with varying cross sections for a zero collision transmission estimator in order to investigate the behavior of the scheme on the free parameters q and Σ_{samp}, and to show that both parameters affect the efficiency of the algorithm. We have chosen an analytically treatable case to gain insight into the main factors affecting optimal parameter settings and conditions of high efficiency gain. For a similar model, a recent article [10] demonstrated numerically the efficiency gain for a single case equivalent in our notation to choosing $q=0$ and $\Sigma_{samp} = \Sigma_{maj}$. We show here that this setting is not the optimal choice.

The transmission test model is a one dimensional system with varying n number of piecewise constant cross sections Σ_i along an equidistantly segmented x path of length L with interval size Δx. The response R is the probability of collisionless transmission with source located at $x=0$ and transmission evaluated at x. With derivations in the Appendix we can state the following:

$$R = e^{-\bar{\Sigma} L} \tag{3.1}$$

with the notation:

$$\bar{\Sigma} = \frac{1}{L}\sum_{i=1}^{n}\Sigma_i \Delta x = \frac{1}{n}\sum_{i=1}^{n}\Sigma_i \tag{3.2}$$

If N number of samples are used, the square of the relative variance r^2 of the estimate reads:

$$r^2 = \frac{1}{N}\left[e^{\frac{q}{1-q}\left(\Sigma_{samp} - 2\bar{\Sigma}\right)L + \frac{\overline{\Sigma^2}L}{\Sigma_{samp}(1-q)}} - 1 \right] \tag{3.3}$$

where we defined the mean squared cross section as

$$\overline{\Sigma^2} = \frac{1}{L}\sum_{i=1}^{n}\Sigma_i^2 \Delta x = \frac{1}{n}\sum_{i=1}^{n}\Sigma_i^2 \tag{3.4}$$

We consider the T computation time proportional to the V number of virtual collisions happening in a history, with the expectation:

$$T \sim E(V) = \frac{1-q}{q}\left(1-e^{-q\Sigma_{samp}L}\right) \tag{3.5}$$

The relative variance will have a minimum if

$$\Sigma_{samp} = \sqrt{\frac{\overline{\Sigma^2}}{q}} \tag{3.6}$$

and the computation time is minimal if $\Sigma_{samp}=0$, thus the efficiency measure, the Figure of Merit (FoM, the higher the value the more efficient the MC algorithm is), defined as

$$FoM = \frac{1}{Tr^2} \tag{3.7}$$

would peak different parameter values as the optimal for either the variance or computing time. Thus we can state that the two free parameters are not interchangeable as suggested by Eq. (3.6) and would affect the efficiency of the calculation in different ways requiring a simultaneous optimization of both parameters. Calculated variances according to Eq.(3.3) and number of collisions according to Eq.(3.5) match very well the corresponding MC simulations as demonstrated in Figure 1.

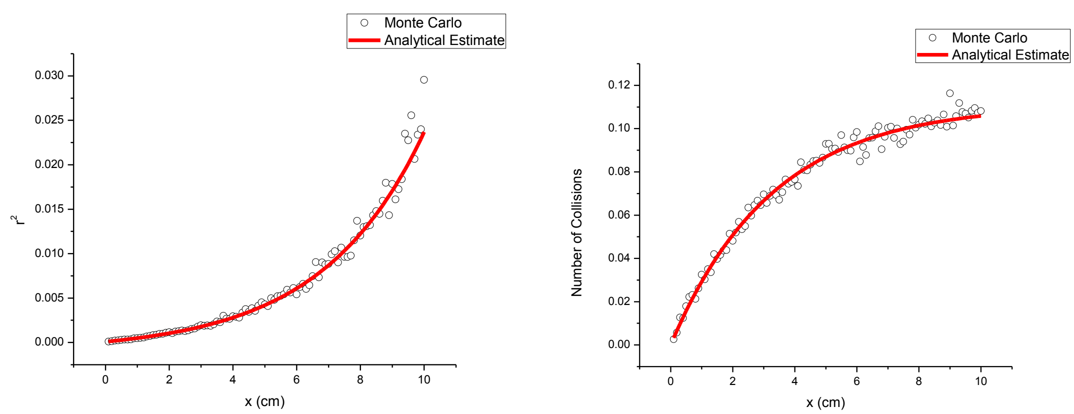

Figure 1. Monte Carlo simulation results and analytical estimates of the square of the relative variance (left) and the number of virtual collisions (right)

FoM optimum cannot be expressed analytically therefore we chose an example with a fixed set of cross sections, with the following parameters: $\Sigma_1=0.48\text{cm}^{-1}$, and $\Sigma_2= \Sigma_3=\ldots =\Sigma_{100}=0.32\text{ cm}^{-1}$, L=10cm, n=100, and carried out the optimizations numerically. We have introduced the parameter p as the ratio of the majorant and the sampling cross section: $p= \Sigma_{samp}/\Sigma_{maj}$. We used the parameters of p=0.7, q=0.9, and 10 000 samples to generate the values of Figure 1.

In Figure 2. we show the optimal p and q parameters at different distances from the source.

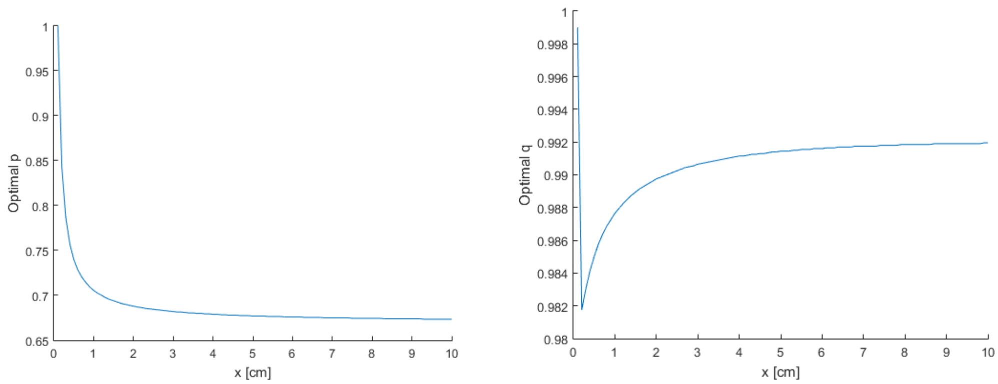

Figure 2. Optimal bias parameters p (left) and q (right) as a function of the distance from the source. Optimal q parameters strongly depend on the actual cross sections. Optimal p parameter is less everywhere than 1, i.e. the majorant cross section is never the optimal sampling cross section

Optimal p parameter values decrease with the distance from the source and seems to vary with the cumulative optical distance. The highest value of p is always less than 1, i.e. the **optimal sampling cross section is lower than the majorant**. Optimal q parameter has an obviously stronger dependence on the actual cross section of a certain location.

The improvement in FoM with the optimal settings can be seen in Figure 3 relative to standard Woodcock tracking.

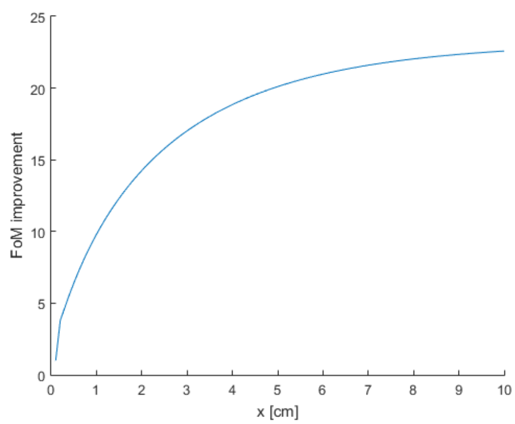

Figure 3. FoM improvement with optimal p and q

Improvement in FoM is strongly dependent on the cross sections of the system in this case a factor of 20 can be shown even though the cross section variations were within a factor of 1.5.

4 Application to Radiotherapy – an Illustration

Brachytherapy is a form of radiotherapy when radioactive sources (or seeds) are placed near or in the tumor in order to maximize the dose delivered to cancer tissues and minimize the radiation exposure of healthy organs [14]. Therapy planning softwares are used for determining optimal positions of the sources and this process requires frequent and fast recalculation of the distribution of delivered dose in a finely segmented spatial mesh with varying cross sections. If the calculation is carried out by MC methods, ray marching would suffer from many surface crossings of the fine mesh, while Woodcock tracking would use the huge cross section of the sources material, although the relevant transport process takes place almost exclusively in the tissue material some 25 times less (in very often applied cases even 800 times less) in total cross section resulting in unnecessarily and impractically small free flight steps.

The code “Monte Carlo SImulator for Brachytherapy Exposure” (M-CSIBE) of our own development used for this illustration is a GPU based MC code specially written for brachytherapy, similar in features to a recently reported code [15] though we have utilized Woodcock tracking instead of ray marching. The code M-CSIBE is built on a MC engine PANNI with verification [16] using MCNP5 [17].

The simulation geometry is a simplified representation of a brachytherapy setup. The system is a water cube (20 x 20 x 20cm) divided into (200 x 200 x 200 =) 8 10^6 segments. The source is of material Ir-192 located at the center of the geometry, is of size 1x1x1mm and emits photons of 380keV energy. Dose is required to be estimated in every space segment. The setup calls for the modified Woodcock tracking: if Ir-192 is present in the system T=1650 s is required to process 10^9 particles on an nVidia GTX 690 graphics card, but if the same simulation is carried out with only water present 15 s would suffice.

With indication towards the optimal values by the one dimensional case study, we have carried out a numerical optimization by repeating the simulation with different q and p using an implementation of the novel method in M-CSIBE. Number of starting particles was 10^{10}. Responses were the released energy per space segment per particle. Figure of Merit results and runtimes are shown in Figure 4 and Table 1.

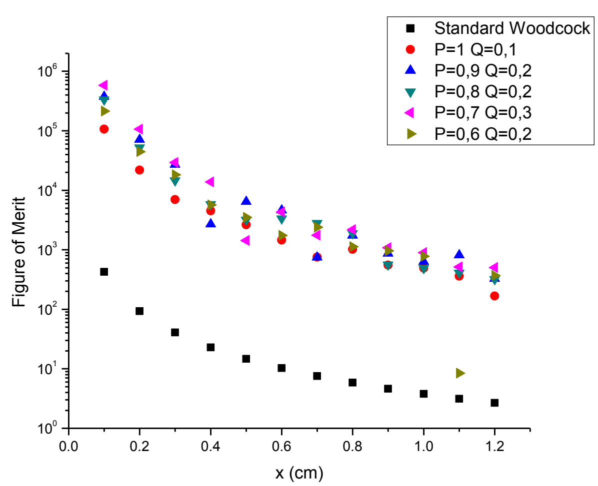

Figure 4. Figure of Merit at different p and q values for the brachytherapy model as a function of the x distance from the source

x (cm)	Standard Woodcock T=16466 s	p=1 q=0.1 T=317 s	p=0.9 q=0.2 T=150 s	p=0.8 q=0.2 T=158s	p=0.7 q=0.3 T=111 s	p=0.6 q=0.2 T=176s
0.1	425.73	106380	375574	334780	579570	214566
0.2	93.11	21858	71363	52215	106346	44669
0.3	40.76	6969	27103	14594	29227	18283
0.4	22.91	4503	2692	5828	13825	5677
0.5	14.71	2626	6462	3177	1436	3516
0.6	10.28	1452	4631	3329	4292	1738
0.7	7.56	750	745	2812	1765	2400
0.8	5.86	1018	1738	1884	2181	1131
0.9	4.62	553	867	563	1088	961
1.0	3.77	490	634	489	895	775
1.1	3.14	361	818	408	513	8
1.2	2.66	167	327	319	501	369

Table 1. Figure of Merit values at different x distances from the source. Column headers contain the corresponding p and q values and running times

Compared to the standard Woodcock algorithm efficiency improvement is vast, at the usual reference evaluation distance of 1 cm from the source the FoM improvement is about a factor of 200. Analyzing the runtimes we see that most of the efficiency improvement is due to the save in computation time (about a factor 100) but also some gain is obtained from the improvement of the squared relative variances (about a factor 2, see Table 2). The computing time save scales favorably with the system size.

x (cm)	Standard Woodcock	p=1 q=0.1	p=0.9 q=0.2	p=0.8 q=0.2	p=0.7 q=0.3	p=0.6 q=0.2
0.1	1.43E-07	2.96E-08	1.77E-08	1.89E-08	1.55E-08	2.64E-08
0.2	6.52E-07	1.44E-07	9.29E-08	1.21E-07	8.43E-08	1.27E-07
0.3	1.49E-06	4.51E-07	2.45E-07	4.34E-07	3.07E-07	3.10E-07
0.4	2.65E-06	6.99E-07	2.46E-06	1.09E-06	6.48E-07	9.99E-07
0.5	4.13E-06	1.20E-06	1.03E-06	1.99E-06	6.24E-06	1.61E-06
0.6	5.91E-06	2.17E-06	1.43E-06	1.90E-06	2.09E-06	3.26E-06
0.7	8.04E-06	4.19E-06	8.90E-06	2.25E-06	5.08E-06	2.36E-06
0.8	1.04E-05	3.09E-06	3.81E-06	3.36E-06	4.11E-06	5.01E-06
0.9	1.32E-05	5.69E-06	7.65E-06	1.12E-05	8.24E-06	5.90E-06
1.0	1.61E-05	6.42E-06	1.04E-05	1.29E-05	1.00E-05	7.31E-06
1.1	1.93E-05	8.71E-06	8.11E-06	1.55E-05	1.75E-05	6.73E-04
1.2	2.28E-05	1.88E-05	2.03E-05	1.98E-05	1.79E-05	1.54E-05

Table 2. Squared relative variances (r^2) with different p and q settings

It is also to notice that the relative variances in Table 2 show some outliers from the smooth pattern expected from the one dimensional example, see e.g. the value at p=0.6, q=0.2 at 1.1 cm. This phenomenon indicates that the estimation may not be robust for all cases given that the sample size was high and the estimated relative variances were well below 1% except for the outlying cases.

5 Discussion and Conclusions

A variant of the Woodcock tracking method has been developed where the sampling cross section may differ from the majorant cross section of the system. The novel method has been proven to be unbiased and gain in efficiency has been shown analytically for a transmission estimator. As an illustration the method has been applied to a geometry inspired by radiotherapy where an efficiency improvement of a factor 200 has been found.

Further investigations may target a position dependent setting of the sampling parameters and the question of estimator robustness.

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8 Appendix

8.1 Proof for inhomogeneous medium

Let us introduce the statistical w weight of a particle, and the K number of collisions occurred throughout its history. Both can be interpreted as a random variable mapping the set of possible outcomes to $\mathbb{R}$ and $\mathbb{N}$ respectively.

According to the rule of total expectation (tower rule), the E expected value of the statistical weight can be written

$$Ew = \sum_{k=0}^{\infty} E\left(w \mid K = k\right) f_K(k)$$

As the distance between collisions is sampled from an exponential distribution, it is trivial, that K follows a Poisson distribution with mean $\Sigma_{samp}L$, where L is the total distance travelled in the medium. f_K denotes the probability mass function of K.

Furthermore, we can apply the tower rule again, conditioning for whether or not a real collision happened. Thus, we obtain:

$$Ew = \sum_{k=0}^{\infty} [E(w \mid K = k, \#real = 0)P(\#real = 0) + E(w \mid K = k, \#real > 0)P(\#real > 0)]\, f_K(k)$$

When a real collision occurs in our simulation, the weight is set to zero meaning that it would not count to the probability of a free path before a collision anymore, therefore the second expectation gives 0. The probability that no real collision occurs out of k is $(1-q)^k$, and the final weight of the particle at the end of the path is the product of $\frac{1-\frac{\Sigma(x_i)}{\Sigma_{samp}}}{1-q}$ for every i:

$$Ew = \sum_{k=0}^{\infty} \left[E\left(\prod_{i=1}^{k} \frac{1 - \frac{\Sigma(x_i)}{\Sigma_{samp}}}{1-q} \right) (1-q)^k \right] f_K(k)$$

Weight-factors $1 - \frac{\Sigma(x_i)}{\Sigma_{samp}}$ are independent, therefore the product and the expectation are interchangeable. As long as the number of collisions (k) is fixed on the interval $[0, L]$, the joint probability density function (PDF) of $x_1, x_2, \dots, x_k$ is a PDF of a uniform distribution (for proof, see [18]). In our case, it means that $\Sigma(\mathrm{x})$ is sampled uniformly on the interval $[0, L]$.

Thus the weight expectation simplifies to

$$Ew = \sum_{k=0}^{\infty} \left[\prod_{i=1}^{k} \left(1 - \frac{\overline{\Sigma}}{\Sigma_{samp}} \right) \right] f_K(k) = \sum_{k=0}^{\infty} \left(1 - \frac{\overline{\Sigma}}{\Sigma_{samp}} \right)^k f_K(k)$$

Where $\overline{\Sigma} = \frac{1}{L} \int_0^L \Sigma(\mathrm{x})\, dx$.

To shorten further calculations we recognize that this formula is very similar to the probability generating function (PGF) of the Poisson distribution (denoted by G), more precisely the expected weight equals the PGF at $1 - \frac{\overline{\Sigma}}{\Sigma_{samp}}$.

Exploiting the PGF it is apparent that

$$Ew = \sum_{k=0}^{\infty} \left(1 - \frac{\overline{\Sigma}}{\Sigma_{samp}} \right)^k f_K(k) = G\left(1 - \frac{\overline{\Sigma}}{\Sigma_{samp}} \right) = e^{\Sigma_{samp} L \left(1 - \frac{\overline{\Sigma}}{\Sigma_{samp}} - 1 \right)} = e^{-\overline{\Sigma} L} = e^{-\int_0^L \Sigma(\mathrm{x}) dx}$$

Our estimate is unbiased.

The proof discussed above shows that our method is a correct way to sample the free path by demonstrating that the expected transmittance is in line with the law of exponential attenuation. As we do not modify the nature of the distribution (we only manipulate with sampling frequency, thus altering the variance), it is sufficient to prove that our estimator is unbiased to justify correctness.

8.2 Relative variance of a transmission estimator with Woodcock tracking

In the case of estimating transmittance we need to calculate the number of transmitted particles M, simulating N total histories. In a Monte Carlo scheme with statistical weights, the transmittance is estimated by the summation of transmitted particle weights over N histories:

$$M = \sum_{n=1}^{N} w^{(n)}$$

The relative variance of our estimate of M is

$$r^2[M] = \frac{1}{N} \left(\frac{E[w^2]}{(E[w])^2} - 1 \right)$$

8.3 Variance for inhomogeneous medium

Let us consider a purely absorbing one dimensional medium with cross section $\Sigma(x)$. Since our estimate is unbiased, the expectation (first moment) is:

$$E[w] = e^{-\overline{\Sigma} L}$$

To calculate the second moment we recall the proof for unbiasedness. One can apply the same reasoning for the expectation of w^2 as for the first moment of w.

$$E[w^2] = \sum_{k=0}^{\infty} \left[E \left(\prod_{i=1}^{k} \left(\frac{1 - \frac{\Sigma(x_i)}{\Sigma_{maj}}}{1 - q} \right)^2 \right) (1 - q)^k \right] f_K(k)$$

With the expansion of the square we get:

$$E[w^2] = \sum_{k=0}^{\infty} \left[\left(\prod_{i=1}^{k} E\left(1 - \frac{\Sigma(x_i)}{\Sigma_{maj}}\right)^2 \right) \frac{1}{(1-q)^k} \right] f_K(k) = \sum_{k=0}^{\infty} \left[\left(\prod_{i=1}^{k} E\left(1 - 2\frac{\Sigma(x_i)}{\Sigma_{maj}} + \frac{\Sigma^2(x_i)}{\Sigma_{maj}{}^2}\right) \right) \frac{1}{(1-q)^k} \right] f_K(k)$$

As before, the expectation is taken according to a uniform distribution:

$$E[w^2] = \sum_{k=0}^{\infty} \left[\left(1 - 2\frac{E[\Sigma(x_i)]}{\Sigma_{maj}} + \frac{E[\Sigma^2(x_i)]}{\Sigma_{maj}{}^2}\right)^k \frac{1}{(1-q)^k} \right] f_K(k)$$

Let $\overline{\Sigma}$ and $\overline{\Sigma^2}$ denote the first and second moment of the cross section distribution, and recognize again, that the formula is the PGF of the Poisson distributed variable K, at a certain point.

$$E[w^2] = G\left(\left(1 - 2\frac{\overline{\Sigma}}{\Sigma_{maj}} + \frac{\overline{\Sigma^2}}{\Sigma_{maj}{}^2}\right) \frac{1}{(1-q)} \right) = exp\left[\left(\frac{1}{1-q} - 1\right) \Sigma_{maj} L - \frac{2\overline{\Sigma} L}{1-q} + \frac{\overline{\Sigma^2} L}{\Sigma_{maj}(1-q)} \right]$$

For the relative variance we get:

$$r^2[M] = \frac{1}{N}\left(\frac{E[w^2]}{(E[w])^2} - 1\right) = \frac{1}{N}\left(exp\left[\frac{q}{1-q}(\Sigma_{maj} - 2\overline{\Sigma})L + \frac{\overline{\Sigma^2} L}{\Sigma_{maj}(1-q)} \right] - 1 \right)$$

8.4 Estimating the runtime of the calculation

As for the simulation time, we assume that it is proportional to the expected number of virtual collisions (denoted by V), which can be written:

$$E[V] = \sum_{k=0}^{\infty} E\,[V|K=k] f_K(k) = \sum_{k=0}^{\infty} \left[\left(\sum_{v=0}^{k-1} (1-q)^v q v \right) + (1-q)^k k \right] f_K(k) =$$

$$= \sum_{k=0}^{\infty} \left[q(1-q) \left(\sum_{v=0}^{k-1} (1-q)^{v-1} v \right) + k(1-q)^k \right] f_K(k)$$

First, we applied the tower rule in order to fix the number of collisions in the expectation. Once the number of collisions is fixed (k), our problem reduces to the question: What is the average number of virtual collisions in a row if a maximum of k collisions are allowed to happen. The chance of getting an exactly v long run of success (virtual collision) out of k Bernoulli trials is $(1-q)^v q$ if $v < k$ and $(1-q)^k$ if $v = k$.

The trick that we use in the next step is the same one which is usually applied to calculate the expected value of a geometric distribution. The reason we factor (1-q) out of the summation is that the remaining expression is the derivative of $-(1-q)^v$ with respect to q.

$$E[V] = \sum_{k=0}^{\infty} \left[q(1-q) \left(\sum_{v=0}^{k-1} \frac{d}{dq} - (1-q)^v \right) + k(1-q)^k \right] f_K(k)$$

Executing the summation of a geometric series and calculating the derivative we get:

$$E[V] = -\sum_{k=0}^{\infty} \frac{1-q}{q}(1-q)^k f_K(k) + \sum_{k=0}^{\infty} \frac{1-q}{q} f_K(k) = \frac{1-q}{q}\left(\sum_{k=0}^{\infty} f_K(k) - \sum_{k=0}^{\infty} (1-q)^k f_K(k) \right)$$

The first sum is easy as it gives 1, due to f_K being a probability mass function. The second sum can be directly connected to the probability generating function, the same way as shown before. The desired expectation then simplifies to:

$$E[V] = \frac{1-q}{q}(1 - G(1-q)) = \frac{1-q}{q}(1 - e^{-q\Sigma_{samp}L})$$

In case of straightforward simulation structures it is safe to assume that the time necessary to execute the calculations (transmit the particles through) is proportional to the average number of virtual collisions. Thus:

$$T \propto E[V] = \frac{1-q}{q}(1 - e^{-q\Sigma_{samp}L})$$