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Variance analysis of Woodcock type tracking

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Abstract - *In this paper, we present an adaptive Woodcock particle tracking method for free path sampling in Monte Carlo neutron and photon transport problems. The proposed algorithm circumvents the major drawbacks of Woodcock's method and provides a low-cost alternative of free path sampling in inhomogeneous media, while being adjustable to the problem at hand. We discuss variance and efficiency analysis for a simple transmission problem, concluding that a priori optimization of the algorithm can be achieved if some information on the cross sections of the problem is known. Comparison of the adaptive and another Woodcock-type tracking algorithm is given in Section 2., showing that optimization requires small effort on part of our adaptive method, moreover, the proposed algorithm is superior in terms of efficiency of the simulation. In Section 3., an application of the adaptive tracking is presented in a brachytherapy setup.*

I. INTRODUCTION

Woodcock type particle tracking has been widely used by Monte Carlo developers since its introduction in neutron transport by Woodcock et al. [1]. This method is based on von Neumann's rejection technique [2], and was independently developed by Skullerud [3] for the plasma physics community. Later, it became a popular method in areas like neutron and ion transport (embedded in SERPENT [4] and MORET [5] codes), radiative transfer [6], computer graphics [7], and medical physics [8], depicted by several names, such as delta-tracking, null-collision algorithm and pseudo scatter. The term "null-collision" is used throughout this paper referring to the event when a sampled tentative collision site is rejected (the particle "scatters" without a change in direction and energy).

The method is intended to overcome difficulties arising from free path sampling in inhomogeneous media. Path length selection is usually achieved by inverting the cumulative distribution function of the path traversed between collisions, which can be a cumbersome task in a non-homogeneous case, especially in complex geometries where retrieving ray-surface intersections are computationally expensive [9]. The principle of Woodcock tracking is to take a fictitious cross section $\Sigma_{maj} \geq max(\Sigma_t(\underline{r}))$ being the majorant of all cross sections in the medium, and sample the probability density function (pdf)

$$f(x) = \Sigma_{maj} e^{-\Sigma_{maj} x} \tag{1}$$

to select path length to a tentative collision. To compensate for sampling with a fictitious cross section Σ_{maj} rather than the real cross section Σ_t, the collision is accepted with probability Σ_t/Σ_{maj} and rejected with probability $1 - \Sigma_t/\Sigma_{maj}$. Mathematical verification of unbiasedness was discussed in [10], and recently generalized to non-constant sampling cross section by Antyufeev [11].

Applying the above method, a meshless (circumventing the necessity of surface-to surface tracking) Monte Carlo particle tracking can be implemented, yet it suffers from a major drawback, also mentioned by [12] [4] [13]: a localized heavy absorber in the medium renders the path length selection ineffective, since the majorant becomes large, causing the algorithm to generate null-collisions unnecessarily often in optically thin regions. Articles addressing the problem agree that introduction of a weighted scheme is necessary, where particle weights (representing a fraction or a bundle of particles) can also become negative, although strategies are slightly different. Here, a weighted (non-analog) simulation means that statistical weight modification accounts for the bias introduced in collision acceptance rate and the distortion of tentative collision site distribution. Carter et al. [14] suggest using non-bounding cross section $C\Sigma_t$ for sampling (with C being a positive function) coupled with a separation of two algorithm branches, distinguished by the sign of $C\Sigma_t - \Sigma_t$. In the positive case, the original Woodcock rejection game is played, but in the negative case, a weight multiplier F is introduced, altering the particle weight to change sign upon a null-collision. As a consequence, negative contributions (weights) are also accepted to the final score. In recent articles by Galtier et al. [15] it is highlighted, that the probability of accepting a collision site is not constrained, thus altering the probability of the null collision event is quite possible. This modification of the algorithm permits the use of non-bounding cross section, also leading to the admittance of negative weights. The article proposes a choice for the acceptance probability which coincides with the one used by Carter et al. [14], making the two algorithms identical apart from the generated distribution of tentative collision sites. Recent research showed [16], that in applications like a radiotherapy problem, a factor of 200 in efficiency gain can be observed by using a simulation with negative weights relative to the standard Woodcock method. Most of the improvement is due to the reduction of computer time, while the method remains stable (producing lower variances) despite the appearance of negative contributions if parameters are carefully set.

This paper also focuses on possible methods of constructing leakage (or transmission) estimators. The most comprehensive literature of transmittance estimators can be found in the computer graphics (CG) field. Woodcock type tracking was introduced in CG community by Raab et al. [17], encouraging the utilization of unbiased MC estimators instead of biased quadrature methods like ray marching. Further contributions were made by Novak et al. [7] by introducing a weighted scheme (only non-negative weights) to Woodcock-tracking, so that the algorithm no longer gives a binary answer for transmittance. It is interesting to note, that the same was concluded in parallel by the nuclear field [13].

II. THEORY

In this section, we present an adaptive Woodcock type free path sampling algorithm, that is not limited by a strictly bounded majorant cross section, thus eliminating the localized heavy absorber problem, and allows an adaptive sampling via two arbitrary chosen parameters q and Σ_{samp}. The algorithm is intended to be a valid alternative for free path sampling in inhomogeneous media, when a cost effective solution is needed as a consequence of complex (meshless) geometry, or procedurally generated media.

The pseudo-code for the proposed method is shown in Algorithm 1. Similar to the derivation of Galtier et al. [15], a new probability q is introduced as an acceptance rate of collisions, however, it remains independently chosen from the sampling cross section Σ_{samp}. Free path selection is carried out by sampling the pdf

$$g(x) = \Sigma_{samp} e^{-\Sigma_{samp} x} \tag{2}$$

where Σ_{samp} is not forced to be a strict majorant.

```
w=1;
while !collided do
    sample Σ_samp e^(−Σ_samp x);
    r = r + Ωx
    if rand() < q then
        collided = true;
        w = w Σ_t(r)/(Σ_samp q);
        r = rand();
        if(r < Σ_c(r)/Σ_t(r)) capture();
        elseif(r < Σ_a(r)/Σ_t(r) + Σ_s(r)/Σ_t(r)) scatter();
        else  fission();
    else
        w = w (1 − Σ_t(r)/Σ_samp)/(1−q);
    end
end
```

Algorithm 1: The adaptive Woodcock tracking algorithm.

The proof of unbiasedness is given in the Appendix.

Parameter q must be restricted to take values from the interval $[0, 1]$, and Σ_{samp} can either be greater or smaller than the maximum of cross sections. Note, that the main advantage of the Woodcock method is thus exploited as the sampling of distance to collisions becomes exceedingly simple, a sample from $g(x)$ is drawn by solving Eq. 3 for x (r denotes a canonically distributed random number).

$$r = 1 - e^{-\Sigma_{samp} x} \tag{3}$$

The major drawback of the original Woodcock algorithm is also eliminated: it is no longer obligatory to choose a majorant cross section for Σ_{samp}, one can even set the desired number of tentative collisions to any level, prior to the calculations. As emphasized in [15], this is only possible because of altering the collision acceptance probability (introducing q).

III. RESULTS AND ANALYSIS

1. A priori estimation of relative error and computer time

A simple transmission problem in one dimensional geometry with non-multiplying medium was chosen to demonstrate a variance analysis of Woodcock type particle tracking. Suppose we have a point source at $\boldsymbol{r_0}$, with particles coming out in direction $\boldsymbol{\Omega}$. The quantity to be estimated is the uncollided flux (transmission) at $\boldsymbol{r_0} + \boldsymbol{\Omega} x$, denoted by $\tau(x, \boldsymbol{\Omega})$. Particles can either be absorbed in the medium or scattered out from the ray, with total cross section Σ_t. A simplified version of the original method (Algorithm 1) that estimates the transmittance is shown in Algorithm 2. With a probabilistic approach (see Appendix), not only the proof of unbiasedness can be given, but variance of the estimation and the expected number of null collisions can also be calculated a priori.

```
τ̂ = 0;
for i=1...N do
    w = 1;
    r = r_0;
    while !collided AND |r − r_0| < x do
        sample Σ_samp e^(−Σ_samp s);
        r = r + Ωs;
        if rand() < q then
            w = 0;
            collided = true;
        else
            w = w (1 − Σ_t(r)/Σ_samp)/(1−q);
        end
    end
    τ̂ = τ̂ + w/N
end
```

Algorithm 2: Transmission (leakage) estimation

The formulas for the relative variance and the expected number of null-collisions (V) will be given here, with the derivation discussed in the Appendix. Let us denote the squared relative error of estimator $\hat{\tau}$ by r^2, and the number of null-collisions by V. Eq. 4 and 5 hold for the squared relative error of $\hat{\tau}$ and the expectation of V.

$$r^2 = \frac{1}{N}\left(exp\left[\frac{1}{1-q}\int_0^x q\left(\Sigma_{samp} - 2\Sigma_t(x')\right) + \frac{\Sigma_t^2(x')}{\Sigma_{samp}} dx'\right] - 1\right) \tag{4}$$

$$E[V] = \frac{1-q}{q}\left(1 - exp\left(-q\Sigma_{samp} x\right)\right) \tag{5}$$

As we have emphasized before, the proposed method aims to be a viable option for free path sampling in cases when geometry is exceedingly complex or somehow it is computationally expensive to fetch the cross sections of a certain location (e.g. the actual cross section is a function of some time-dependent calculation). Notice in Algorithm 2, that there is only one line, where the cross section of the current location should be retrieved, and that is when a null-collision occurs. Therefore, the number of null-collisions can be a fair measure of computation time, i.e.

$$T \propto \frac{1-q}{q}\left(1 - exp\left(-q\Sigma_{samp}x\right)\right). \tag{6}$$

In a more general sense, one may try to find some connection between parameters (q, Σ_{samp}) and computer time T, then carry out the optimization accordingly, based on the example we present in the next section. Now, we only wish to draw attention to the fact that given enough information about the problem, the computation time and the relative error of the estimation can be approximated prior to any particle tracking calculation. Eq. 4 suggests, that sufficient information is provided by the knowledge of the first and second moment of the cross section distribution as the only variables depending on x are Σ_t and Σ_t^2. Of course, exact calculation of the first moment solves the original problem itself (transmission is uniquely determined), however, approximate knowledge may also be advantageous.

We implemented the above method (Algorithm 2) in a C++ computer code to check Eq. 4 and 5 against simulation results. The output of the simulation were the average weights and squared weights of particles reaching x, and the average number of null-collisions occured to these particles. Fig. 1 shows the cross sections of the example problem. Note, that sampling is chosen to be below the majorant cross section, permitting negative contributions to the final score $\hat{\tau}$. The total cross section of the problem is given by

$$\Sigma_t(x) = 0.2 + 0.2\ sinc\,[4(x-3)] \tag{7}$$

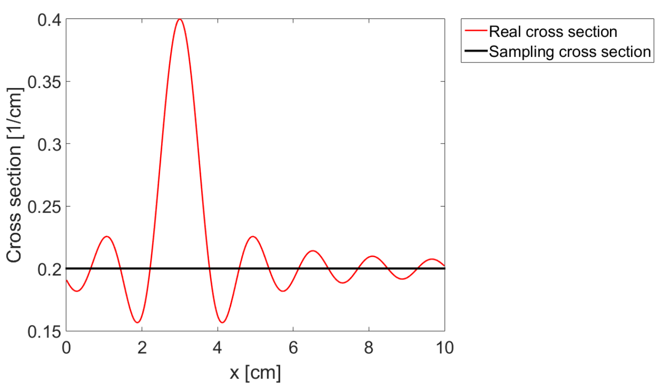

Fig. 1. Cross sections in the example problem

A priori calculation of variance and expected number of null-collisions are compared with Monte Carlo simulation results, shown in Fig. 2. The example problem was analyzed by setting $q = 0.3$ and $\Sigma_{samp} = 0.2cm^{-1}$. During the simulation 10^5 particle histories were generated.

2. A numerical optimization study

This section shows a numerical optimization of the adaptive Woodcock algorithm for a transmission problem. Optimization is based on Equations 4 and 5, which implies that the calculation of the exact optimal choice of parameters requires more effort, than solving the problem itself. Nevertheless, it will be shown that optimal parameters can indeed be found, thus if an approximation on the cross sections is available, it may improve the efficiency of the algorithm greatly.

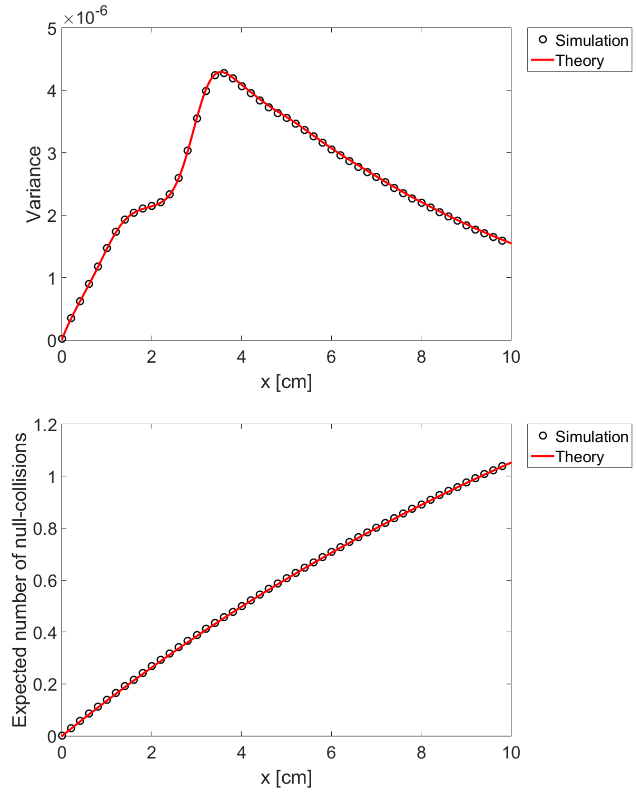

Fig. 2. Verification of a priori relative error and computation time calculation

An interesting version of the Woodcock-type tracking algorithms is compared to our adaptive tracking in this section. The reference algorithm developed by Carter et al. [14] proposes a different sampling than our method, as it does not take a constant sampling cross section, but uses the pdf of

$$C(x)\Sigma(x)e^{-C(x)\Sigma(x)} \tag{8}$$

to select path length to a tentative collision. Note, that in this case the distances between collisions are not independent, identically distributed random variables (although they are still exponentially distributed). Thus, the generated stochastic process is not a Poisson process, and the reasoning shown in the Appendix can not be applied here. In fact, the proof of unbiasedness can still be formulated elegantly as in [14], but calculation of relative error and number of null-collisions requires numerical evaluation of many convolutions. The computational cost is suspected to be large compared to the complexity of the problem, which might be the reason why the authors did not discuss analytical formulas for predicting variance and computer time. There is an optimization shown in [14] that uses simulation results of runs with different C constants. This investigation is only shown for a collision estimator, the optimum is found at around $C = 3.625$. As we are to compare transmission (leakage) estimators, we will reconstruct the optimization of Carter's algorithm as well.

Introduce the efficiency of the simulation by the usual definition:

$$FoM = \frac{1}{r^2 T}, \tag{9}$$

i.e. the Figure of Merit (FoM) being inversely proportional to the squared relative error of the estimation and the time spent on calculating the estimation. Two simulation scheme may be compared by their FoM values: greater FoM means that the same precision (r^2) may be realized with less effort, or by spending the same amount of time the simulation achieves smaller relative error.

Again, consider the computation time proportional to the number of cross section fetches, in other words, let us assume, that most of the computer time is spent on retrieving the cross section of the location (executing the "where am I?" routine). Looking at Equations 4 and 5, the Figure of Merit of the adaptive Woodcock method can be calculated as a function of Σ_{samp} and q:

$$\begin{aligned} &FoM(q, \Sigma_{samp}) = \\ &\left\{ \frac{1}{N} \left(exp\left[\frac{1}{1-q} \int_0^x q\left(\Sigma_{samp} - 2\Sigma(x')\right) + \frac{\Sigma^2(x')}{\Sigma_{samp}} dx' \right] - 1 \right) \cdot \right. \\ &\left. \qquad \cdot \frac{1-q}{q} \left(1 - exp\left(-q\Sigma_{samp} x\right)\right) \right\}^{-1} \end{aligned} \tag{10}$$

Unfortunately, global extrema of FoM can not be expressed analytically as $\frac{\partial FoM}{\partial q} = 0$ and $\frac{\partial FoM}{\partial \Sigma_{samp}} = 0$ lead to transcendent equations. Therefore, we must turn to some numerical method. To illustrate that optimal parameters can indeed be found, Fig. 3 shows how the efficiency of the calculation depend on the choice of parameters Σ_{samp} and q.

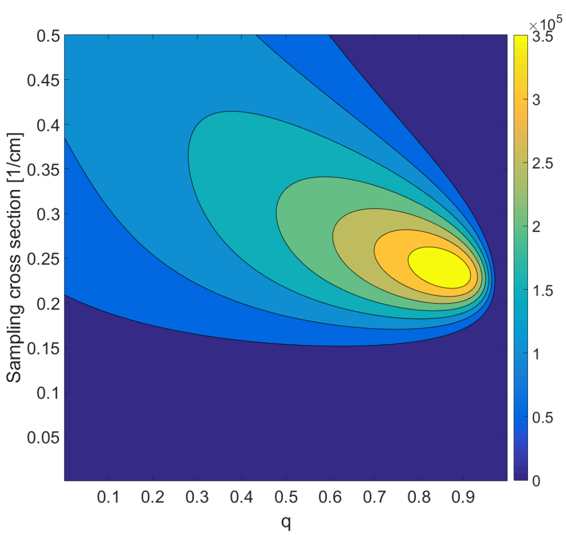

Fig. 3. Figure of Merit as a function of parameters Σ_{samp} and q. Optimization of the adaptive Woodcock algorithm can be carried out numerically, the maximum of FoM found at $\Sigma_{samp} = 0.236\ cm^{-1}$ and $q = 0.868$

Fig. 3 also shows, that with larger q than optimal, FoM quickly drops in the region around the optimal Σ_{samp}, FoM value is also very sensitive of altering Σ_{samp} in the vicinity of the optimum. As a consequence, q must be chosen with caution, in real applications we suggest it to be an underestimation of the suspected optimal value. Then, some uncertainty of the initial information can not cause too much trouble, as our guess for the optimum is farther from the region of large gradients.

In order to find a fair comparison, Carter's algorithm [14] should also be optimized to transmission estimation. Fig. 4 shows how an optimum is found in this case. The top two graphs contain simulation results for the relative error of the estimation and the expected number of cross section fetches required to achieve this error at different C settings. The bottom graph shows calculated FoM values according to Eq. 9, with maximum located at around $C = 2$. Table I suggests

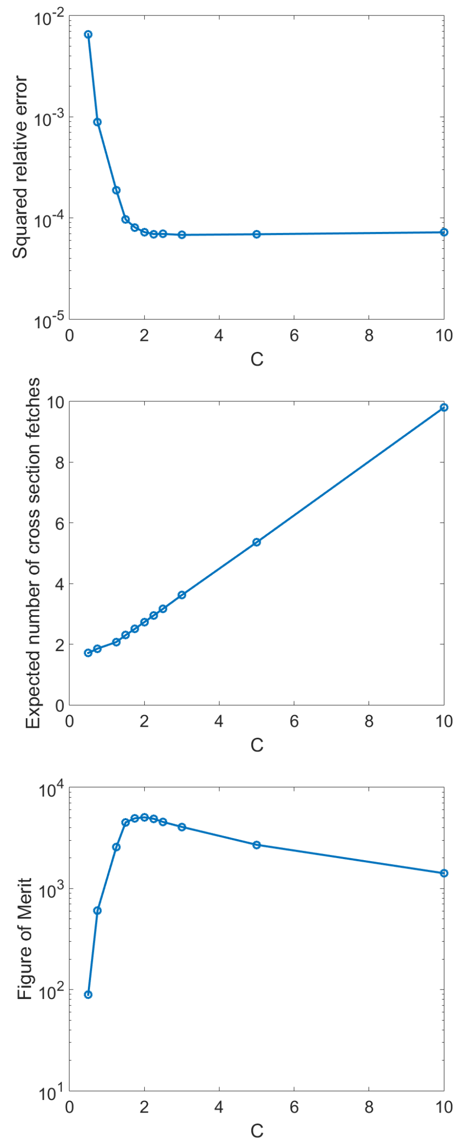

Fig. 4. Optimization of Carter's Woodcock tracking for transmission estimation

that with C between 1.5-2-5, variation of FoM is less than 10%, therefore $C = 2$ will be used as an optimum.

C	FoM
0.5	89
0.75	606
1.25	2554
1.5	4505
1.75	4949
2	5054
2.25	4891
2.5	4547
3	4066
5	2704
10	1415

TABLE I. Efficiency as a function of parameter C in Carter's algorithm [14] for transmission estimator

As Table II shows, the main difference between the two methods is that our adaptive Woodcock tracking uses the original cross sections very rarely, which was the original intention of the algorithm design. Notice, that Carter's algorithm must retrieve the cross section of the current position whenever a free path is sampled regardless of the outcome of the collision (being a real or virtual(null-) collision). With the same number of particle histories generated, the achieved relative error is a bit greater, but the save in computer time can compensate for it, if it is indeed proportional to the number of cross section fetches. In this case, efficiency increase is almost an order of magnitude relative to Carter's method.

	r^2	Average number of cross section fetches	FoM
Carter's algorithm $C = 2$	$7.24{\cdot}10^{-5}$	2.73	5054
Adaptive Woodcock $q = 0.868$ $\Sigma_{samp} = 0.236\ cm^{-1}$	$1.93{\cdot}10^{-4}$	0.13	39857

TABLE II. Comparison of two Woodcock type tracking algorithm for transmission estimation. The proposed adaptive algorithm outperforms the optimally set reference algorithm almost an order of magnitude in efficiency measure.

3. Application in radiotherapy

In Section 2. we showed how a numerical optimization could be carried out for a simple transmission problem when analytic solution is available. Based on Equations 4 and 5, an approximation of the optimal parameters may also be obtained even when the information on the distribution of cross sections is incomplete, e.g. only the approximate average or the maximum/minimum of cross sections are known in advance. Regarding more complex problems, finding an optimum is not so easy, it can very well be as cumbersome task as finding a solution to the problem itself.

We analyzed the behavior of our adaptive Woodcock algorithm in a brachytherapy setup, fully described in [16]. Brachytherapy is a form of radiotherapy, when cancer cells are targeted by radiation from brachytherapic seeds, placed near the tumor. At the treatment planning phase, distribution of absorbed dose in the target volume and in healthy tissues is of interest, which may be calculated via Monte Carlo simulation. Using a Woodcock maximum cross section technique for free path sampling would degrade the efficiency of the simulation, as particle tracking would take impractically small steps following the distribution determined by the maximum of cross sections, i.e. the source material. Our investigation [16] showed, that indeed, a factor of 200 can be found in efficiency increase by using the adaptive scheme, mostly due to the save in computation time.

We found that the efficiency measure (Figure of Merit - FoM) strongly depends on parameter q as the absorbed dose is of question, and FoM seems to slowly vary with sampling cross section Σ_{samp} at lower collision acceptance rates ($q < 0.1$). However, choosing the optimal parameters require Σ_{samp} to be lower than the maximum cross section as optimal q parameter is in the region where efficiency dependence on Σ_{samp} is stronger. Recall, that this in line with the conclusions of the 1D example problem, thus it may not be unexpected at all. As an illustration, let us consider the absorbed dose at position $x = 0.5\ cm$ (with a point source at the origin, and the problem fully described in [16]). Fig. 5 shows the Figure of Merit of the absorbed dose estimation as a function of collision acceptance probability q.

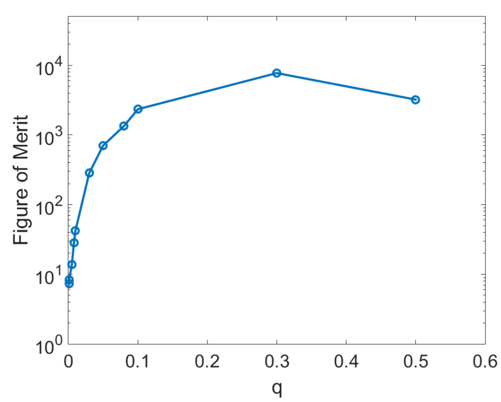

Fig. 5. Efficiency as a function of collision acceptance rate

Fig. 5 points out, that with $q \to 0$ efficiency rapidly declines due to the infrequent sampling of real collisions, when energy transfer may occur (contribution to the absorbed dose is made). Increasing q may therefore be beneficial, but as the chosen collision acceptance rate gets larger, the majority of real collisions tends to happen nearer the source and as a consequence, contribution to the absorbed dose come from fewer particles and with greater variance. At $x = 0.5\ cm$,

Fig. 5 shows that an optimal q is reached at $q \approx 0.3$. As shown in [16], at different positions, different optimal values can be determined, thus position dependent setting of parameters must be considered. Future research should focus on energy dependent problems as well.

IV. CONCLUSIONS

In this paper, an adaptive Woodcock tracking algorithm was presented. The method is constructed to be a fast and reliable option for free path sampling in inhomogeneous media. The presented algorithm does not suffer from the drawback of the standard Woodcock method and provides an adaptive sampling that can be tailored to the Monte Carlo problem via two sampling parameters. Variance analysis was shown for a transmission problem, highlighting the fact that a priori optimization of parameters is possible, when some information on the cross sections is known. Verification of the variance calculation was presented by comparing to simulation results, with the derivation of formulas in the Appendix. A comparison of Carter's delta tracking algorithm [14] and the adaptive Woodcock method showed that our algorithm can be especially favorable in cases when retrieving the cross section at a certain position is associated with high computational cost. Investigations on the behavior of the method in a brachytherapy setup pointed out, that efficiency increase may be vast even in real problems, a factor of 200 has been found as an improvement of FoM relative to the standard Woodcock tracking.

V. FUTURE WORK

Variants of Woodcock's original particle tracking method have been developed by several disciplines in the Monte Carlo community, focusing on the applicability of the algorithm to special problems where the standard tracking would be otherwise inefficient. These publications offer unique choice of parameters that can be traced back to q (the collision acceptance probability) and Σ_{samp} (sampling cross section). It can be shown, that in general, none of the suggested parameters are optimal to a problem. It turns out that one could construct a generalized algorithm that includes all of these special cases, which is in fact partly covered by the adaptive method presented in this paper. Some additional effort should be made however to develop a truly general scheme, consider for example position dependent parameters $q(x)$ and $\Sigma_{samp}(x)$. Some preliminary results show that sampling with a varying cross section may improve efficiency even further. Future research may include zero variance schemes and variance analysis of other type estimators e.g. collision estimators.

APPENDIX

The Appendix presents derivations of Eq. 4 and 5. The reasoning is based on previous work published in [16].

Proof for inhomogeneous media

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 expected value of the statistical weight can be written

$$E[w] = \sum_{k=0}^{\infty} E[w \mid K = k] f_K(k). \tag{A.1}$$

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 traveled 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. Introducing the number of virtual collisions V, we obtain:

$$E[w] = \sum_{k=0}^{\infty} E[w \mid K = k, V = k] P(V = k) + E[w \mid K = k, V < k] P(V < k) f_K(k). \tag{A.2}$$

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

$$\frac{1 - \frac{\Sigma(x_i)}{\Sigma_{samp}}}{1-q} \tag{A.3}$$

for every i:

$$E[w] = \sum_{k=0}^{\infty} E\left[\prod_{i=1}^{k} \frac{1 - \frac{\Sigma(x_i)}{\Sigma_{samp}}}{1-q}\right] (1-q)^k f_K(k). \tag{A.4}$$

Weight-factors $1 - \dfrac{\Sigma(x_i)}{\Sigma_{samp}}$ 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 of $x_1, x_2, , x_k$ is a pdf of a uniform distribution (for proof, see [18]). In our case, it means that $\Sigma(x)$ is sampled uniformly on the interval $[0, L]$. Thus the weight expectation simplifies to

$$E[w] = \sum_{k=0}^{\infty} \left(\prod_{i=1}^{k} 1 - \frac{\overline{\Sigma}}{\Sigma_{samp}}\right) f_K(k) = \sum_{k=0}^{\infty} \left(1 - \frac{\overline{\Sigma}}{\Sigma_{samp}}\right)^k f_K(k) \tag{A.5}$$

where $\overline{\Sigma} = \dfrac{1}{L}\displaystyle\int_0^L \Sigma(x)dx$. To shorten further calculations we recognize that this formula is very similar to the probability generating function (PGF) of the Poisson distribution, more precisely the expected weight equals the PGF at $1 - \dfrac{\overline{\Sigma}}{\Sigma_{samp}}$. Exploiting the PGF it is apparent that

$$E[w] = \sum_{k=0}^{\infty} \left(1 - \frac{\overline{\Sigma}}{\Sigma_{samp}}\right)^k f_K(k) = G\left(1 - \frac{\overline{\Sigma}}{\Sigma_{samp}}\right) = e^{\Sigma_{samp}L\left(1 - \frac{\overline{\Sigma}}{\Sigma_{samp}} - 1\right)} = e^{-\overline{\Sigma}L}. \tag{A.6}$$

Our estimate is unbiased. The proof discussed above shows that our method is a correct way to sample a particle's 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.

Relative error 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:

$$M = \sum_{n=1}^{N} w^{(n)}. \tag{A.7}$$

The squared relative error of our estimate of M is

$$r^2[M] = \frac{1}{N}\left(\frac{E\left[w^2\right]}{(E[w])^2} - 1\right). \tag{A.8}$$

Relative error 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:

$$E[w] = e^{-\overline{\Sigma}L}. \tag{A.9}$$

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.

$$E\left[w^2\right] = \sum_{k=0}^{\infty} E\left[\prod_{i=1}^{k}\left(1 - \frac{\Sigma(x_i)}{\Sigma_{samp}}\right)^2\right]\frac{1}{(1-q)^k} f_K(k). \tag{A.10}$$

With the expansion of the square we get:

$$E\left[w^2\right] = \sum_{k=0}^{\infty}\prod_{i=1}^{k} E\left[1 - 2\frac{\Sigma(x_i)}{\Sigma_{samp}} + \frac{\Sigma^2(x_i)}{\Sigma^2_{samp}}\right]\frac{1}{(1-q)^k} f_K(k). \tag{A.11}$$

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

$$E\left[w^2\right] = \sum_{k=0}^{\infty}\left(1 - 2\frac{\overline{\Sigma}}{\Sigma_{samp}} + \frac{\overline{\Sigma^2}}{\Sigma^2_{samp}}\right)^k \frac{1}{(1-q)^k} f_K(k) \tag{A.12}$$

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

$$E\left[w^2\right] = G\left(\left(1 - 2\frac{\overline{\Sigma}}{\Sigma_{samp}} + \frac{\overline{\Sigma^2}}{\Sigma^2_{samp}}\right)\frac{1}{1-q}\right) = \\ = e^{\left(\frac{1}{1-q}-1\right)\Sigma_{samp}L - \frac{2\overline{\Sigma}L}{1-q} + \frac{\overline{\Sigma^2}L}{\Sigma_{samp}(1-q)}}. \tag{A.13}$$

For the squared relative error we get:

$$r^2[M] = \frac{1}{N}\left(\frac{E\left[w^2\right]}{(E[w])^2} - 1\right) = \frac{1}{N}\left(e^{\frac{q}{1-q}\left(\Sigma_{samp} - 2\overline{\Sigma}\right)L + \frac{\overline{\Sigma^2}L}{\Sigma_{samp}(1-q)}} - 1\right). \tag{A.14}$$

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:

$$E[V] = \sum_{k=0}^{\infty} E\left[V|K=k\right] f_K(k) = \\ = \sum_{k=0}^{\infty}\left(\sum_{v=0}^{k-1}(1-q)^v qv + (1-q)^k k\right) f_K(k) = \\ = \sum_{k=0}^{\infty}\left(q(1-q)\sum_{v=0}^{k-1}(1-q)^{v-1}v + k(1-q)^k\right) f_K(k). \tag{A.15}$$

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, what 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:

$$E[V] = \sum_{k=0}^{\infty}\left[q(1-q)\left(\sum_{v=0}^{k-1}\frac{d}{dq} - (1-q)^v\right) + k(1-q)^k\right] f_K(k). \tag{A.16}$$

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

$$E[V] = -\sum_{k=0}^{\infty}\frac{1-q}{q}(1-q)^k f_K(k) + \sum_{k=0}^{\infty}\frac{1-q}{q} f_K(k) = \\ = \frac{1-q}{q}\left(\sum_{k=0}^{\infty} f_K(k) - \sum_{k=0}^{\infty}(1-q)^k f_K(k)\right). \tag{A.17}$$

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:

$$E[V] = \frac{1-q}{q}\left(1 - G(1-q)\right) = \frac{1-q}{q}\left(1 - e^{-q\Sigma_{samp}L}\right). \tag{A.18}$$

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:

$$T \propto E[V] = \frac{1-q}{q}\left(1 - e^{-q\Sigma_{samp}L}\right). \tag{A.19}$$

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