Causes of multimodality of efficiency gain distributions in accelerated Monte Carlo based dose calculations for brachytherapy planning using correlated sampling

Daniel Deniz

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Summary

Fixed-collision correlated sampling for Monte Carlo (MC) simulations is a method which can be used in order to shorten the simulation time for brachytherapy treatment planning in a 3D patient geometry. The increased efficiency compared to conventional MC simulation is measured by efficiency gain. However, a previous study showed that, in some cases, PDFs (probability density functions) of estimates of the efficiency gain, simulated using resampling and other MC methods, were multimodal with values below 1. This means that the method was less effective than conventional sampling for these cases. The aims of this thesis were to trace the causes of the multimodal distributions and to propose techniques to mitigate the problem caused by photons with high statistical weights.

Two simulation environments were used for the study case, a homogeneous and a heterogeneous environment. The homogenous environment consisted of a water sphere with the radius 100mm. For the heterogeneous environment a cylindrical block of tungsten alloy (diameter 15 mm, height 2.5 mm) was placed in the water sphere. The sphere was divided into an array of cubic voxels of size 2.5 mm x 2.5 mm x 2.5 mm for dose calculations. A photon source was positioned in the middle of the water sphere and emitted photons with the energy 400 keV.
It was found that the low values and multimodal PDFs for the efficiency gain estimates originated from photons depositing high values of energy in some voxels in the heterogeneous environment. The high energy deposits were due to extremely high statistical weights of photons interacting repeatedly in the highly attenuating tungsten cylinder. When photon histories contributing to the rare events of high energy deposits (outliers) were removed, the PDFs became uni-modal and efficiency gain increased. However, removing outliers will cause results to be biased calling for other techniques to handle the problem with high statistical weights.

One way to resolve the problem in the current implementation of the fixed-collision correlated sampling scheme in PTRAN (the MC code used) could be to split photons with high statistical weights into several photons with the same sum weight as the initial photon. The splitting of photons will result in more time consuming simulations in areas with high attenuation coefficients, which may not be the areas of interest. This could be resolved by using Russian roulette, eliminating some of the photons with high statistical weight in such areas.
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Abbreviations and symbols

ANL  Analogue
CPU  Central Processing Unit
CT  Computed Tomography
ETL  Expected Track Length
HCF  Heterogeneity Correction Factor
MC  Monte Carlo
MCPT  Monte Carlo Photon Transport
PDF  Probability Density Function

X,Y  Batch averages of scored $D_{\text{het}}$ and $\Delta D_c$, respectively. X and Y are random variables.

$S_X^2, S_Y^2$  Estimators of $V(X)$ and $V(Y)$, where $V(X)$ and $V(Y)$ are variances of X and Y respectively.

G  Efficiency gain estimator (a random variable estimating $\gamma$)

$x, y, s_X^2, s_Y^2, g$  Samples from X, Y, $S_X^2, S_Y^2$ and G respectively.

$\bar{D}$  Estimated value of absorbed dose in a voxel

$\bar{x}, \bar{y}$  Averages of $N_V$ sample values from x and y, respectively.

$\bar{W}, W$  Statistical weights for photons within the heterogeneous and homogeneous environments respectively.

$N_H$  Number of histories in the run, $N_H=10^8$.

$N_B$  Number of sample values present in x and y, $N_B=25 000$.

$N_S$  Number of histories in one batch (size of batch), $N_S=4000$.

$N_V$  Number of sample values $x_i$ and $y_i$ used to calculate $s_X^2$ and $s_Y^2$, respectively. $N_V=3 000$

$\gamma$  Efficiency gain (a number derived from parameters of two distributions)
1. Introduction

1.1 Background

Brachytherapy is a form of radiation therapy where the radiation source is placed inside or in direct contact with the target volume of interest. This form of radiation treatment is often used to treat localized prostate and cervical cancers. The absorbed dose, which describes the level of irradiation of tissue, decreases with increasing distance from the source. The preparation of a dose plan is a non trivial task as both the primary photons, whose amount is decreased by the inverse square law and exponential attenuation, and the scattered photons contribute to the absorbed dose.

According to Nath et al [1], values of absorbed doses are often taken from previous Monte Carlo (MC) simulations of absorbed dose to water in homogeneous water phantoms to plan the brachytherapy treatment of a patient. Because every individual is different with body tissue compositions deviating from that of water, the usage of pre-calculated values for absorbed dose to water results in less accurate dose calculations for treatment planning. The effect of seed-to-seed attenuation is also ignored; it considerably influences absorbed doses to patients during low dose-rate radiation treatments.
Individual patient planning with MC simulation based on information of the patient anatomy and tissue compositions from CT (computerized tomography) images is one way to increase the accuracy. The problem is that it is CPU (central processing unit) demanding and time consuming to achieve results with sufficient statistical precision. A large number of photon histories are needed.

In order for MC simulations to be used in clinics for individual treatment planning, a simulation time less than a few minutes is desirable. To reach this goal, variance reduction techniques could be used to decrease the variance and make it possible to run the MC simulation under much shorter time.

Hedtjärn et al [2] showed that correlated sampling can be used as a variance reduction technique for accelerated MC based dose calculations for brachytherapy. In their work, the Monte Carlo Photon-Transport (MCPT) simulation code PTRAN with an extension to perform fixed-collision correlated sampling was used to run the simulations. The photon histories were generated in a homogeneous environment and, simultaneously, their paths re-used for the heterogeneous environment. Weight correction factors were used to reflect the presence of heterogeneities. It was reported in [2] that the efficiency using the correlated MC simulation technique with PTRAN was increased for most of the voxels in the heterogeneous geometry, but for some of the voxels it was appreciably decreased, cf. Figure 1.
1.2 Aims of work

Malušek et al [3], focused on finding confidence intervals for the efficiency gain reported in [2]. It was found that the PDF (probability density function) for the estimated values of efficiency gain was multimodal for some voxels whereas uni-modal, Gaussian distributions were expected. The multimodality made it hard to simply predict confidence intervals of the calculated efficiency gain.

The aims of this work were (i) to explain the findings by Malušek et al [3] by analyzing particle tracks causing multimodal PDFs of efficiency gain and (ii) to propose techniques that mitigate the problem caused by photons with high statistical weights.
2. Theory

2.1 Physics of photon transport

When a photon moves within a medium, there are several different interactions which can occur. With ionizing radiation, the most important interactions of photons with energies up to 400 keV are photoelectric absorption, incoherent- and coherent scattering.

Photoelectric absorption is when the photon gets absorbed by an atom or a molecule and an electron is emitted from the inner atomic shell. An electron from a higher energy level will in turn take the emitted electron’s place. The energy thereby released is emitted as a characteristic x-ray or an Auger or Coster-Kronig electron. The probability of photoelectric absorption depends both on the atomic number of the medium with which the photon interacts but also on the photon energy. Highest probability for absorption is when the medium has large atomic number and the photon has low energy.

Incoherent scattering, also called Compton scattering, is when a photon gets scattered against an atomic electron. The electron gains energy and recoils from the atomic shell leaving behind a positive ion. The scattered photon loses some of its energy and takes a new direction of motion.
In coherent scattering, a photon is elastically scattered by the whole atom. The emitted photon has approximately the same energy as the initial photon due to the, in comparison, large mass of the atom. Notably, the only difference between the initial and the emitted photon is the direction of motion.

2.2 Generating photon histories using random numbers

2.2.1 Analogue (ANL) simulation

Using ANL simulations, photon trajectories are simulated using random numbers to select values from probability distributions according to the laws of physics. First the photon energy and the direction of motion is selected. Next, a point of interaction for the photon is chosen from the frequency function \( p(x) = \mu e^{-\mu x} \) (1) where \( p(x) \) is the probability per unit length that the photon interacts after traveling a distance \( x \); \( \mu \) is the linear attenuation coefficient. The type of interaction is chosen according to the probabilities \( \sigma_{PE}/\mu, \sigma_{inc}/\mu \) and \( \sigma_{coh}/\mu \) for photoelectric absorption, incoherent and coherent scattering. If photoelectric absorption occurs, the trajectory is finished and a new trajectory is generated. If instead scattering occurs, a new direction of motion and energy of the photon are selected according to the appropriate differential scattering cross section. Thereafter, a new point of interaction is chosen and the same steps are repeated until the photon is either absorbed in a photoelectric absorption or escapes the volume of interest.

(1) This formula is valid for a homogeneous medium only.
2.2.2 Non ANL simulation

The difference between ANL and non ANL simulation of photon trajectories is that the latter one uses fictitious probability and frequency functions when generating the trajectories. In order to compensate for the bias this causes, a correction weight $W_j$ is assigned to the photon. The weight is given by the quotient between the true and false probability densities for interacting according to a given sequence of interactions. Non-analogue simulations are used either to achieve variance reduction or to reduce simulation time in order to increase efficiency (see 2.4 and 2.5).

2.2.3 Description of photon histories

A photon history (photon trajectory) can be described by a sequence of parameters $\alpha_j=(r_j, \Omega_j, E_j)$, where $r_j$ is the position of the photon at the $j$:th interaction, $\Omega_j$ is its direction of motion and $E_j$ its energy directly after collision $j$. For photons emitted from the source, $j = 0$.

The histories were randomly constructed from two different probability functions, one for the emission of photons from the source and one for the transition between interaction points. When a primary photon was simulated, $\alpha$ was chosen from the source term $Q$ (number of photons emitted per unit volume from the source with the energy $E$ and direction vector $\Omega$ per unit energy and solid angle). Otherwise, the probability density for the transition from $\alpha_j$ to $\alpha_{j+1}$ is given by a transition kernel $K$, described in [4].
2.3 Scoring of mean absorbed dose to voxels in the phantom

The simulated photon histories are used to estimate a quantity of interest using a scoring function. Here the mean absorbed dose in a voxel is considered. Let $D_{\text{hom}}(\mathbf{z})$ be the mean absorbed dose in voxel $\Delta V$ with the position vector $\mathbf{z}$ in a homogeneous medium. $D_{\text{hom}}(\mathbf{z})$ can be estimated by taking the average of the dose contributions scored in each of $N$ generated photon histories.

$$
D_{\text{hom}}(\mathbf{z}) = \frac{1}{N} \sum_{i=1}^{N} \sum_{j=0}^{N_i} W_{i,j} f(\alpha_{i,j} | \mathbf{z}) 
$$

(1)

$f(\alpha_{i,j} | \mathbf{z})$ is the dose-scoring function for the $j$:th collision of the photon history $i$ and gives the dose contribution of collision $\alpha_{i,j}$ at the location $\mathbf{z}$. $W_{i,j}$ is a weight which compensates for the bias when using non-analogue simulation (see 2.2.2). When using analogue simulation $W_{i,j} = 1$. $N$ is the number of histories and $N_i$ is the number of collisions in each history. The same method can be used to estimate $D_{\text{het}}(\mathbf{z})$ for a heterogeneous environment. The corresponding weight and dose-scoring function are written $\tilde{W}$ and $\tilde{f}(\alpha_{i,j} | \mathbf{z})$. It is noticed that the quantity in equation (1) as based on $N$ photon histories, is a stochastic quantity due to the stochastic nature of the interaction processes.

2.3.1 Analogue (ANL) scoring – ANL estimator

When using ANL scoring, a simulated collision only gives a non-zero contribution to the energy imparted when it occurs within the voxel of interest. The ANL contribution depends on the energies of the incoming and outgoing photon. Thus the dose-scoring function of the ANL estimator is dependent on both $\alpha_j$ and $\alpha_{j+1}$ and is given by equation (2) (equation (14) in [2]):

$$
f(\Delta V, \alpha_j; \alpha_{j+1}) = \frac{E_j - E_{j+1}}{\rho V \Delta V} 
$$

(2)

$\rho V$ is the density of the medium inside the volume $\Delta V$. 
2.3.2 Non analogue scoring - ETL (expected track length) estimator

With analogue scoring, the probability of a non-zero score to a given voxel is small. To increase the probability of scoring in a voxel, analytical calculations can be added to the dose scoring function. ETL scoring is such a method which gives a non-zero contribution to all voxels intersected by a projection of the photon path even beyond the actual point of interaction. The dose scoring function of the ETL estimator is given by equation (3) (equation (15) in [2]):

\[ f(\Delta V, \alpha_j) = \frac{E_j e^{-\mu l_r} (1-e^{-\mu \Delta l}) (\mu_{en} \rho)}{\rho \Delta V} \]  

(3)

The dose scoring function is used for each voxel traversed by the projection of the photon path; \( f=0 \) if the projected photon trajectory misses the voxel. Here, \( \mu \) is the linear attenuation coefficient, \( \mu_{en} \) the energy absorption coefficient, \( \rho \) the mass density of the medium inside the voxel, \( \Delta V \) the volume of the voxel, \( l \) the distance from \( r_j \) to the proximal-most intersection of \( \Delta V \) in the direction of \( \Omega_j \) and \( \Delta l \) the length of this ray contained within \( \Delta V \).

2.4 Variance reduction techniques

2.4.1 Using non analogue sampling of photons

Non-analogue sampling of photon histories can be used to reduce the variance of the scored quantities or to speed up the calculations, thus increasing the efficiency of the dose calculations (see section 2.5). A commonly used method is to prevent photons from being absorbed (survival biasing). Another method is to force the photons to interact within the volume of interest (forced collision). Both methods can be shown to decrease the variance but, on the other hand, the histories will never end because the photons can neither be absorbed nor escape from the volume of interest. The weight correction factor to account for survival biasing and forced collision is continuously reduced in subsequent interactions. To force the histories to an end, Russian roulette is used when the weight has decreased below a given value. With a set probability, the photon is killed in the next interaction. Photons which by chance survive the Russian roulette continue their trajectories with an increased weight.
2.4.2 Correlated sampling

To further reduce the variance of the estimate in a heterogeneous environment, correlated sampling may be used. Let $D_{\text{hom}}$ be the absorbed dose in a voxel when having a homogeneous environment, in our study case the emitting source embedded in a sphere of water (see section 3.1). In the case when a tungsten cylinder was introduced into the water sphere, a heterogeneous environment was created and the absorbed dose called $D_{\text{het}}$. $\Delta D$ is defined as the difference between $D_{\text{het}}$ and $D_{\text{hom}}$.

$$\Delta D = D_{\text{het}} - D_{\text{hom}} \quad (5)$$

$D_{\text{het}}$ can then be calculated from values of $D_{\text{hom}}$ using a heterogeneous correction factor (HCF) according to:

$$D_{\text{het}} = HCF \cdot D_{\text{hom}} \quad (6)$$

where $HCF = 1 + \Delta D / D_{\text{hom}}$, which is evident from equation (5).

Using MC simulation, $D_{\text{hom}}$ in a voxel can be estimated by using equation (1). The same applies to MC simulation of $D_{\text{het}}$ in the heterogeneous environment. For small changes, estimates of $D_{\text{het}}$ and $D_{\text{hom}}$ need to be very precise in order to get statistically reliable estimates of $\Delta D$. This would require a large number of simulated photon histories, which would be time consuming.

To solve this problem, correlated sampling can be used. $D_{\text{hom}}$ is then pre-calculated with very high precision using MC simulation so that the variance ($V(D_{\text{hom}})$) is negligible. Then a set of $N$ photon histories is generated in the homogeneous environment. A corresponding set of histories in the heterogeneous environment is created by ray-tracing photons through the same interaction points as in the homogeneous medium with weights assigned to the photons to correct for the heterogeneous environment.
The variance of an estimator of $D_{\text{het}}$, derived using equation (6) and denoted $\bar{D}_{\text{het}}^*$ can then be written as:

$$V(\bar{D}_{\text{het}}^*) = V(\Delta\bar{D}^c) + V(\bar{D}_{\text{hom}}^c) \approx V(\Delta\bar{D}^c)$$

(7)

where $\Delta\bar{D}^c = \bar{D}_{\text{het}}^c - \bar{D}_{\text{hom}}^c$ is estimated using equation (11). Index c indicates that correlated sampling is used. The variance of $\Delta\bar{D}^c$ is:

$$V(\Delta\bar{D}^c) = V(\bar{D}_{\text{het}}^c) + V(\bar{D}_{\text{hom}}^c) - 2COV(\bar{D}_{\text{het}}^c, \bar{D}_{\text{hom}}^c)$$

(8)

Ideally $\bar{D}_{\text{het}}^c$ and $\bar{D}_{\text{hom}}^c$ are strongly correlated, that is when the difference in the homogeneous and heterogeneous environment is small. Strong correlation gives the covariance a positive value, leading to a decrease in the variance for $\Delta\bar{D}^c$. The covariance term is limited by:

$$COV(\bar{D}_{\text{het}}^c, \bar{D}_{\text{hom}}^c) \leq \sqrt{V(\bar{D}_{\text{het}}^c)V(\bar{D}_{\text{hom}}^c)}$$

(9)

If the correlation coefficient equals 1, equality holds for equation (9). Equation (8) can thus be written as

$$V(\Delta\bar{D}^c) = V(\bar{D}_{\text{het}}^c) + V(\bar{D}_{\text{hom}}^c) - 2\sqrt{V(\bar{D}_{\text{het}}^c)V(\bar{D}_{\text{hom}}^c)} = (\sqrt{V(\bar{D}_{\text{het}}^c)} - \sqrt{V(\bar{D}_{\text{hom}}^c)})^2$$

(10)

This means that under some special circumstances $V(\Delta\bar{D}^c)$ can be quite small and sometimes 0 (if $V(\bar{D}_{\text{het}}^c) = V(\bar{D}_{\text{hom}}^c)$). However, large differences in the scored doses in the two environments can lead to a decorrelation and a negative covariance. This could lead to an increased $V(\Delta\bar{D}^c)$ and ultimately an efficiency decrease when using correlated sampling.

The difference in scored doses is written:

$$\Delta\bar{D}^c = \frac{1}{N} \sum_{i=1}^{N} \sum_{j=0}^{N_i} (\bar{W}_{ij} \bar{f}_{ij} - \bar{W}_{ij} f_{ij})$$

(11)

Where $N$ is the number of histories, $N_i$ is the number of interactions in history $i$. $\bar{W}_{ij}$ and $f_{ij}$ are the statistical weight and the dose-scoring function for the $j$:th interaction in history $i$ for
the homogeneous environment. \( \hat{W}_{i,j} \) and \( \tilde{f}_{i,j} \) are the same as above but for the heterogeneous environment. If analogue sampling is used, \( W_{i,j} = 1 \).

The statistical weight \( (W_j) \) is updated after an interaction, i.e., the photon is given new statistical weight \( (W_{j+1}) \). The statistical weights for the heterogeneous environment (due to use of fixed interaction points in the homogeneous and heterogeneous environments) were updated according to:

\[
\hat{W}_{j+1} = \hat{W}_j \left( \frac{\mu(E_j; \mathbf{r}_{j+1})}{\mu(E_j)} e^{-\lambda_{j,j+1}} \right) \left( 1 - e^{-\mu(E_j) t_{\text{max}}} \right) \left( 1 - \frac{\sigma_{\text{PE}}(E_j; \mathbf{r}_{j+1})}{\mu(E_j)} \right) (12)
\]

Where \( \mu(E_j; \mathbf{r}_{j+1}) \) is the linear attenuation coefficient for a photon with the energy \( E_j \) in the medium given by the location \( \mathbf{r}_{j+1} \). The same goes for the macroscopic cross section of the photoelectric effect \( \sigma_{\text{PE}} \). \( \mu(E_j) \) is always the linear attenuation coefficient for the photon with the energy \( E_j \) in water (homogeneous environment). \( t_{\text{max}} \) is the maximum distance from \( \mathbf{r}_j \) to the boundary of the phantom in the direction of the photon movement after interaction \( j \). \( \lambda_{j,j+1} \) is the radiological distance (see equation (22)) between interactions \( j \) and \( j+1 \). The factors in the second and third parenthesis are the weight correction factors to compensate for forced collisions and survival biasing respectively. More detailed description is given in [3].

When the photon moves in the homogeneous environment, the first factor after the previous weight, \( \hat{W}_j \), in equation (12) equals 1. The homogeneous weight (to account for use of fictitious frequency functions in the homogeneous environment) is updated according to:

\[
W_{j+1} = W_j (1 - e^{-\mu(E_j) t_{\text{max}}}) (1 - \frac{\sigma_{\text{PE}}(E_j)}{\mu(E_j)}) (13)
\]

The factor in the first parenthesis accounts for use of forced collision and that in the second parenthesis for use of survival biasing.

(2) The history index \( i \) is omitted for brevity.
2.5 Efficiency and efficiency gain

The efficiency of a MC simulation is defined as:

\[
\text{Efficiency} = \frac{1}{t \cdot V} \quad (14)
\]

Where \( t \) is the simulation time and \( V \) is the variance of the scored quantity. The efficiency gain (\( \gamma \)) using correlated sampling can be written as the ratio between the efficiencies using uncorrelated and correlated sampling respectively.

\[
\gamma = \frac{\frac{1}{t_c \cdot V_c}}{\frac{1}{t \cdot V}} = \frac{t + V}{t_c + V_c} \quad (15)
\]

Figure 1: A scatter plot of the efficiency gain estimator as a function of HCF. The figure is taken from [3]

Figure 1 above shows that the efficiency gain was low (below 1) for voxels with HCF below 0.6. These voxels were located behind the tungsten shielding which lowered the absorbed dose in this region. The reduced efficiency comes from an increased variance when \( \bar{D}_{het} \) deviates substantially from \( \bar{D}_{hom} \) as mentioned in section 2.4.
3. Method

3.1 The PTRAN MC code and study case

The MCPT (Monte Carlo Photon Transport) code PTRAN version 8.0 was developed by professor Jeffrey Williamson and collaborators, see Williamson [5]. In the study case, fixed collision non-ANL MC simulations with survival biasing and forced collisions were used to simulate the average absorbed dose to each voxel in the three dimensional (3D) voxel array using ETL scoring. The homogenous environment consisted of a water sphere with a radius of 100 mm and a point source located at the center of the sphere. The source emitted 400 keV photons. For the heterogeneous environment a cylindrical block of tungsten alloy, with diameter 15mm and height 2.5mm, was placed with its center 10mm from of the source, see Figure 3. The tungsten alloy had a mass density of 17g/cm³ and consisted of elements with the weight fractions: Fe 8.18%, Ni 16.86% and W 74.96%.

![Figure 3: The heterogeneous environment for the simulation. The point source was positioned in the center of the geometry (a water sphere of radius 100 mm) with a cylindrical block of tungsten (diameter 15 mm, height 2.5 mm) placed with its center 10mm from the source. An array of uniform size voxels (2.5mm x 2.5mm x 2.5mm) was a part of the geometry.](image-url)
Figure 4: The location of 28 voxels on the central axis. $i_v$ denotes the voxel index which ranges from 1 to 28. Figure taken from [3].

3.2 Data handling

3.2.1 Output files

Correlated and non-correlated production versions of the PTRAN code were modified to provide additional information about photon histories and absorbed doses to voxels via history-specific and voxel-specific output files.

Voxel-specific output files were tables with the history number in the first column and the scored $\bar{\Delta}D^c, \bar{D}_{hom}^c$ or $\bar{D}_{het}$ in the second column, see Table 1. Each file corresponded to a specific voxel. Only non-zero contributions to the scored quantity were listed. The number of rows ranged between 380 000 and 14 000 000 depending on the number of contributions. Voxels closer to the point source typically received more contributions.
The total number of simulated histories was \( N_H = 10^8 \) and the simulation times of the conventional and correlated sampling simulations were 2.09 and 2.20 hours, respectively.

<table>
<thead>
<tr>
<th>History number</th>
<th>Energy deposited, keV</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>14</td>
</tr>
<tr>
<td>23</td>
<td>155</td>
</tr>
<tr>
<td>45</td>
<td>23</td>
</tr>
<tr>
<td>47</td>
<td>90</td>
</tr>
</tbody>
</table>

Table 1: A voxel-specific output file contained two columns. One with history numbers and the other with corresponding scored quantity (\( \Delta D^r, D^c_{\text{hom}} \) or \( D_{\text{het}} \)).

The history-specific output files contained information about each interaction \( j \) within history number \( i \). The information represented in the history-specific output files for the correlated sampling scheme is seen in Table 2.

<table>
<thead>
<tr>
<th>History number (i)</th>
<th>( r_i ) – point of interaction</th>
<th>( \Omega_i ) – direction of motion after interaction</th>
<th>voxel indicies</th>
<th>( W_i ) – hom. weight</th>
<th>( W_{ij} ) – het. weight</th>
<th>Medium</th>
<th>Interaction number (j)</th>
<th>( E_i ) photon energy [keV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>2449</td>
<td>xyz</td>
<td>xyz</td>
<td>xyz</td>
<td>10000</td>
<td>10000</td>
<td>1</td>
<td>0</td>
<td>400</td>
</tr>
<tr>
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<td>xyz</td>
<td>xyz</td>
<td>6529</td>
<td>66708</td>
<td>2</td>
<td>1</td>
<td>302</td>
</tr>
<tr>
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<td>xyz</td>
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<td>xyz</td>
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<td>2728</td>
<td>1</td>
<td>2</td>
<td>150</td>
</tr>
</tbody>
</table>

Table 2: The structure for a history-specific output file. \( x \ y \ z \) stands for 3 values, one along each direction axis (3D). Media 1 and 2 correspond to water and the tungsten alloy, respectively. These files were used to investigate changes of statistical weights of photons in correlated sampling.
3.2.2 Calculation of batch averages and efficiency gain

Let $\Delta d^c=(\Delta d^c_1, \ldots, \Delta d^c_{NH})$ and $d_{het}=(d_{het_1}, \ldots, d_{het_{NH}})$ be samples of random vectors $\Delta D^c=(\Delta D^c_1, \ldots, \Delta D^c_{NH})$ (correlated sampling) and $D_{het}=(D_{het_1}, \ldots, D_{het_{NH}})$ (uncorrelated sampling), respectively. These random vectors contain $NH$ identically distributed random variables that correspond to all contributions from all histories to a particular voxel during an MC run. The sample values $\Delta d^c_i$ and $d_{het_i}$ were the ones represented in the voxel-specific output files where $i$ stands for the history number. If a certain history $i$ was not present in the voxel-specific output file, the sample value in position $i$ was set to 0. The $NH$ values of $\Delta d^c$ and $d_{het}$ were grouped into $NB=25 000$ smaller groups with $NS=4 000$ members.

\begin{align*}
\Delta d^c & \rightarrow x \\
\text{Average for } NS \text{ values} & \\
\text{Average for } NS \text{ values} & \\
\text{Average for } NS \text{ values} & \\
\end{align*}

Figure 2: Procedure of batch averaging for $\Delta d^c$ resulting in $x$ which can be seen as a new sample with values from the random variable $X$.

For each group, an average (here called batch average) $x_i$ or $y_i$ where $1 \leq i \leq NB$, was calculated as:

\begin{align*}
x_i &= \frac{1}{NS} \sqrt{t_c} \sum_{j=1}^{NS} d_{het,NS(i-1)+j} \\
y_i &= \frac{1}{NS} \sqrt{t_c} \sum_{j=1}^{NS} \Delta d^c_{NS(i-1)+j}
\end{align*}

$t$ and $t_c$ were simulation times for the uncorrelated and the correlated runs, respectively. Both simulation times were supposed to be non-stochastic. Clearly these times fluctuated for short runs, nevertheless it is always possible to make the runs long enough so that these fluctuations
are negligible. \( x=(x_1, \ldots, x_{N_B}) \) and \( y=(y_1, \ldots, y_{N_B}) \) was seen as samples taken from random variables \( X \) and \( Y \). By including the simulation time into \( X \) and \( Y \), the efficiency gain in equation (15) was calculated using the ratio of variances \( V(X) \) and \( V(Y) \) only.

Assume that \( \Delta D^c \) and \( D_{het} \) are independent random variables with a finite mean value and variance. The finite mean value was evident because of the physical nature of the problem. There cannot be more energy imparted to the voxel than was emitted from the point source. It is also reasonable to assume that the variance was finite. Then according to the statistical central limit theorem, corresponding \( X \) and \( Y \) were approximately Gaussian distributed, if \( N_S \) was chosen sufficiently large.

Variances of \( X \) and \( Y \) were estimated via estimators \( S^2_X \) and \( S^2_Y \), respectively. Corresponding samples were calculated as

\[
S^2_{k,X} = \frac{1}{N_V} \sum_{i=1}^{N_V} (x_i - \bar{x})^2 \quad (17.1)
\]

\[
S^2_{k,Y} = \frac{1}{N_V} \sum_{i=1}^{N_V} (y_i - \bar{y})^2 \quad (17.2)
\]

where \( N_V=3\,000 \), \( \bar{x} \) and \( \bar{y} \) are averages defined as \( \sum_{i=1}^{N_V} \frac{x_i}{N_V} \) and \( \sum_{i=1}^{N_V} \frac{y_i}{N_V} \), respectively.

In previous work, [3], 50,000 values of both \( S^2_X \) and \( S^2_Y \) were used to construct empirical probability density functions. In order to draw that many values in the current implementation, resampling was used. \( N_V \) values from \( X \) and \( Y \) were randomly taken with replacement for the calculation of each sample in equation (17.1) and (17.2), respectively. This procedure was repeated 50,000 times in order to construct empirical probability density functions of \( S^2_X \) and \( S^2_Y \) for one voxel.
The efficiency gain, $\gamma$, defined in equation (15) was estimated via an estimator $G$ defined as [3]:

$$G = \frac{s^2_z}{s^2_\gamma} \quad (18)$$

The efficiency gain estimator $G$ is a random variable. For brevity and where confusion cannot occur, we sometimes omit the word “estimator” and talk about the efficiency gain $G$. Nevertheless, the reader should bear in mind that the “true” efficiency gain $\gamma$ is defined in equation (15). A sample $g$ of the efficiency gain was calculated by dividing samples $s^2_z$ by $s^2_\gamma$ according to equation (18).

### 3.2.3 Data processing

Calculations were performed with Matlab version 7.7. Owing to memory constraints of the available computer, Matlab scripts used for reading PTRAN output files and subsequent simulations were compiled with Matlab’s MEX compiler. This also significantly increased the speed of calculations.

The samples $x$, $y$, $s^2_x$, $s^2_\gamma$ and $g$ were stored as vectors, this made it easier for Matlab to handle all the values due to its matrix based environment. Program loops were used to evaluate equations (16) and (17) as described in section 3.2.2, corresponding computer code is in appendix 8.3. The vector of estimates $g$ was calculated via element-wise division of vectors $s^2_x$ and $s^2_\gamma$. 
4. Results

Samples of x, y, $s_X^2$, $s_Y^2$ and g were used to construct empirical probability density functions of corresponding random variables X, Y, $S_X^2$, $S_Y^2$ and G. These functions are often called PDF estimates in this work. Figures in this section show their non-normalized versions (the number of samples is each histogram-bin).

4.1 Non-normality of batch averages

As defined in section (3.2.2), X and Y are random variables that represent estimated absorbed doses from uncorrelated and correlated data. The PDFs of X and Y were expected to approach, according to the statistical central limit theorem, a Gaussian distribution. The estimated PDFs of random variables X and Y for voxels 6, 14, 20 and 24 are displayed below:

Figure 5: Non-normalized estimates of PDFs of random variables X and Y with batch size 4 000. Each histogram was filled with 25 000 values. Values of X and Y are given in units of $p$, which is a function of internal PTRAN units of time and absorbed dose. The description of internal PTRAN units was not available to the author.
Figure 5 shows that the PDFs for the random variable X (heterogeneous uncorrelated case, left column) all have approximately Gaussian distributions. The PDFs for the random variable Y (correlated dose difference, right column) however appear to be non-Gaussian distributions with outliers.

### 4.2 Multimodal PDFs of variance estimators

Variances of random variables X and Y was estimated according to equation (17:1) and (17:2). Unimodal distributions with Gaussian shape were expected. Frequency functions of variance estimators $S^2_X$ and $S^2_Y$ for voxels 6, 14, 20 and 24 are displayed below, Figure 6.

Figure 6: Non-normalized estimates of PDFs for random variables $S^2_X$ and $S^2_Y$, Values of X and Y are given in units of p, which is a function of internal PTRAN units of time and absorbed dose. The description of internal PTRAN units was not available to the author.

Figure 6 shows that the variance estimators did not behave as expected; most of them had multimodal distributions.
4.3 Multimodal efficiency gain estimator

For normally distributed batch averages, the efficiency gain $G$ in equation (18) has a transformed F-distribution [3]. The estimates of the PDFs of $G$ for voxels 6, 14, 20 and 24 are displayed below, Figure 7.

![PDF of G](image)

Figure 7: Un-normalized estimates of PDFs for $G$ where $g$ is the dimensionless efficiency gain and $N$ is the number of counts in a histogram bin.

Figure 7 shows that for voxels 20 and 24, the estimated PDFs for $G$ are multimodal with some samples lower than 1, an efficiency decrease.
4.4 Tracing multimodality in the efficiency gain distribution

In order to find out why the estimates of the PDFs for the efficiency gain $G$ were multimodal, the modes with larger values than the main mode in the variance estimates of $Y$ were removed. Every value which exceeded a set limit in the estimated variance $S_Y^2$ was given an infinite value. The infinite value appeared in $G$ as the value zero, due to the division in equation (18). The process is shown for voxel 20:

![PDF of $S_Y^2$ vs. PDF of $G$](image)

Figure 8: High value peeks in the PDF of random variable $S_Y^2$ are removed for voxel 20. The resulting non-normalized estimates of the PDFs for the random variable $G$ is displayed to the right.

Figure 8 shows that the low value peaks in the PDF of $G$ were the direct result of the high value peaks in the PDF of $S_Y^2$. 

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The high value samples of $S^2_Y$ were traced back to $y$ with equation (16). The high values of $s^2_Y$ was a result of samples from the random variable $Y$ that greatly deviated from a batch average $\bar{y}$. In order to find the batches causing the high values in $s^2_Y$, a temporary vector was created with the same length as the number of batches present in $y$. Every time a batch was present in the random combination of batches leading to a value in $s^2_Y$ higher that the set limit, the value of the position in the temporary vector with the same number as the batch from $y$ is added by 1. This means that the temporary vector was a chart of how many times a batch in a certain position was present in high sample values of $S^2_Y$. For voxels 20, 23, 24 and 25, the vector with batches present in large sample values of $S^2_Y$ is seen below.

Figure 9: Number of times that batches are present in the batch combinations which result in large $S^2_Y$ values. The single most present batch is zoomed (right row).
One batch value seemed to appear more frequently than all the others when a large value was generated for each voxel. Further investigation (zoom, the right column) showed that it was batch number 6 124 for voxel 20 (containing an average of the histories 24 496 000 to 24 500 000). For voxels 23 to 25 it was batch number 16 572 (containing an average of the histories 66 284 000 to 66 284 400).

When analyzing the histories contained within batch number 6 125 for voxel 20 and batch number 16 572 for voxels 23 to 25, one specific history contributed with scored values which greatly deviated from the rest in each voxel. The deviating histories for each voxel are listed below in Table 3.

<table>
<thead>
<tr>
<th>Voxel number</th>
<th>History number</th>
<th>Stored value for given history number in $\Delta d^c$</th>
<th>Mean value of all photon history contributions (zero and non-zero) in $\Delta d^c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>24 496 187</td>
<td>370 680</td>
<td>-775</td>
</tr>
<tr>
<td>23</td>
<td>66 287 223</td>
<td>411 890</td>
<td>-538</td>
</tr>
<tr>
<td>24</td>
<td>66 287 223</td>
<td>398 800</td>
<td>-481</td>
</tr>
<tr>
<td>25</td>
<td>66 287 223</td>
<td>342 100</td>
<td>-430</td>
</tr>
</tbody>
</table>

Table 3: Stored and mean values for voxels from figure 9 at some specific histories.

The reason for the multimodal PDF of $S_X^2$ in voxel 14 (figure 6) was the opposite to that of $S_Y^2$. Low sample values in $x$ due to missing histories in $\tilde{d}_{het}$ (zero filling, see section 3.2.2) caused high variance estimates due to values much lower than the batch average $\bar{x}$. This finding was only an artifact of a non-complete voxel-specific output file for voxel 14 from PTRAN and had no significant meaning for the interpretation of the results.
4.5 Removal of high value histories

In order to find out how histories with high scored values affected $S_Y^2$ and G, these histories were removed from the voxel-specific output files for some voxels.

History number 66 287 223 (see Table 3) was removed from the voxel specific output files for voxels 23, 24 and 25. The resulting PDF estimates for $S_Y^2$ and G are shown below:

![PDF estimates](image)

Figure 10: Un-normalized estimates of PDFs for variance estimate $S_Y^2$ (to the left) and efficiency gain G (to the right) for voxels 23 to 25 after removal of the values for history number 66 287 223 (see Table 3).

The multimodality was no longer present in the PDF estimates of neither $S_Y^2$ nor G. The value of G in Figure 10 is also always greater than one. We can draw the conclusion that history number 66 287 223 was responsible for the multimodality and efficiency decrease in voxels 23, 24 and 25 when batch averaging and resampling was used.
History number 24 496 187 (see Table 3) was removed from the voxel-specific output files for voxel 20. The resulting PDF estimates for $S_Y^2$ and G are shown in figure 11.

![Graph showing variance of delta D cor after modification for voxel 20](image)

![Graph showing resulting efficiency gain for voxel 20](image)

Figure 11: Non-normalized estimates of PDFs for variance estimate $S_Y^2$ (on the top) and efficiency gain estimator G (on the bottom) for voxel 20 after removal of the value for history number 24 496 187.

In all four voxels, the removal of the high-value histories resulted in more well behaved PDF estimates for both $S_Y^2$ and G. Also the values below 1 in G were no longer present. Therefore the estimated efficiency when using the previous described methods was improved for all four voxels when the high value histories were removed. Although the removal of the high value histories leaded to a higher estimated efficiency gain, this was not a possible measure to take because it will bias the result of the simulation.
4.6 Tracing scored doses with high values

According to equation (11) the scored dose difference $\Delta D^c$ depends on both statistical weights and dose scoring functions for the homogeneous and heterogeneous environments. Table 4 shows the PTRAN history-specific output file for histories 24 496 187 and 24 496 317.

<table>
<thead>
<tr>
<th>History number</th>
<th>$W$</th>
<th>$\bar{W}$</th>
<th>Medium</th>
<th>Interaction number</th>
<th>Photon energy [keV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>24496187</td>
<td>10000</td>
<td>10000</td>
<td>1</td>
<td>0</td>
<td>400</td>
</tr>
<tr>
<td>24496187</td>
<td>6529</td>
<td>66708</td>
<td>2</td>
<td>1</td>
<td>302</td>
</tr>
<tr>
<td>24496187</td>
<td>4353</td>
<td>484685</td>
<td>2</td>
<td>2</td>
<td>298</td>
</tr>
<tr>
<td>24496187</td>
<td>2931</td>
<td>2744876</td>
<td>2</td>
<td>3</td>
<td>288</td>
</tr>
<tr>
<td>24496187</td>
<td>2013</td>
<td>864836</td>
<td>1</td>
<td>4</td>
<td>254</td>
</tr>
<tr>
<td>24496317</td>
<td>10000</td>
<td>10000</td>
<td>1</td>
<td>0</td>
<td>400</td>
</tr>
<tr>
<td>24496317</td>
<td>6529</td>
<td>59600</td>
<td>2</td>
<td>1</td>
<td>163</td>
</tr>
<tr>
<td>24496317</td>
<td>5173</td>
<td>2728</td>
<td>1</td>
<td>2</td>
<td>150</td>
</tr>
</tbody>
</table>

Table 4: Table with some chosen values from the PTRAN history-specific output file for histories 24 496 187 and 24 496 317. $W$ and $\bar{W}$ are the homogeneous and the heterogeneous weights. Medium 1 was water and medium 2 was the tungsten alloy.
Table 4 shows that the heterogeneous weight increased as the homogeneous weight decreased when a photon interacted within the tungsten cylinder (medium no. 2). Equation (11) shows that this contributed to a higher scored value for $\Delta D^c$. In the case of history number 24 496 187, the photon interacted 3 times inside the cylindrical disk. This resulted in an increase of the heterogeneous weight with about 300 times.

To trace the large increase in weight, equation (12) and (13) were investigated further. They were rewritten as:

$$W_{j+1}/W_j = \left( \frac{\mu(E_j; r_{j+1})}{\mu(E_j)} e^{-\lambda_j r_{j+1} / \mu(E_j)} \right) \left( 1 - e^{-\mu(E_j) t_{max}} \right) \left( 1 - \frac{\sigma_{PE}(E_j; r_{j+1})}{\mu(E_j)} \right)$$ (19)

$$W_{j+1}/W_j = \left( 1 - e^{-\mu(E_j) t_{max}} \right) \left( 1 - \frac{\sigma_{PE}(E_j)}{\mu(E_j)} \right)$$ (20)

In order for the heterogeneous statistical weight to increase, equation (19) needed to be greater than 1. The 3 factors of equation (19) were analyzed separately.

$$0 < 1 - e^{-\mu(E_j) t_{max}} < 1$$

This was a result of $\mu(E_j)$ and $t_{max}$ being positive finite values.

$$0 < \left( \frac{\sigma_{PE}(E_j; r_{j+1})}{\mu(E_j; r_{j+1})} \right) < 1 \iff 0 < \left( 1 - \frac{\sigma_{PE}(E_j; r_{j+1})}{\mu(E_j; r_{j+1})} \right) < 1$$

This goes for both water and the tungsten alloy, since $\mu$ is the sum of cross sections of all interaction types ($\mu=\sigma_{PE}+ \sigma_{INCOH}+ \sigma_{COH}$).

The only difference between the weight correction equations for the homogeneous and the heterogeneous environment (equation (19) and (20)) that could have a value greater than 1 was the factor:

$$W_{C_{hom,het}} = \frac{\mu(E; r_{j+1}) e^{-\lambda_j r_{j+1}}}{\mu(E_j) e^{-\mu(E_j) t_{max}}}$$ (21)
The radiological distance $\lambda_{j,j+1}$ was calculated as the line integral:

$$\lambda_{j,j+1} = \int_0^t \mu(\mathbf{r}_j + S\mathbf{O}_j) dS$$  \hspace{1cm} (22)

t was the distance between the two points $\mathbf{r}_j$ and $\mathbf{r}_{j+1}$ in the 3D environment. When a photon passed the distance $|\mathbf{r}_j - \mathbf{r}_{j+1}|$ within the same medium, the corresponding radiological distance $\lambda_{j,j+1} = \mu(E_j;\mathbf{r}_j)|\mathbf{r}_j - \mathbf{r}_{j+1}|$. If the medium was water $WC_{hom,het} = 1$, this gave equation (19) a value below 1. But if the medium was not water, equation (21) was written as:

$$WC_{hom,het} = \frac{\mu(E_j;\mathbf{r}_{j+1})}{\mu(E_j)} e^{-|\mathbf{r}_j - \mathbf{r}_{j+1}|}[\mu(E_j;\mathbf{r}_j) - \mu(E_j)]$$

$e^{-|\mathbf{r}_j - \mathbf{r}_{j+1}|}[\mu(E_j;\mathbf{r}_j) - \mu(E_j)] < 1$, at the same time $\frac{\mu(E_j;\mathbf{r}_{j+1})}{\mu(E_j)} > 1$ for the tungsten alloy. Thus the variables deciding the value of $WC_{hom,het}$ are the photon energy and the distance between two interactions. The mean distance between two interactions (mean free path) for a photon in water is written as $\frac{1}{\mu(E_j)}$.

Figure 12 shows that the mean free path for a photon in water varies between 0cm and 10cm for energies between 0keV and 400keV. In the PTRAN version used for this study case the photons were forced to interact within the water sphere. The forced interaction makes the
mean distance between two interactions somewhat smaller than shown in figure 12. The photon histories were generated in the homogeneous water environment as mentioned earlier.

In the figure below \( W_{\text{hom,het}} \) inside the tungsten cylinder is shown for different distances between two interactions as a function of photon energy.

Figure 13. The value of \( W_{\text{hom,het}} \) is shown for different distances between two photon interactions within the tungsten cylinder as a function of photon energy.

Figure 13 shows that the value of \( W_{\text{hom,het}} \) can exceed 1. In our case, this was more likely for high photon energies and short photon free paths. In order to find out if the values of \( W_{\text{hom,het}} \) were large enough to make \( \bar{W}_{j+1} > \bar{W}_j \), the weight correction factor in equation (19) was calculated for different cases. \( t_{\text{max}} \) was set to the value 8cm in order to investigate if \( W_{\text{hom,het}} \) could result in \( \bar{W}_{j+1} > \bar{W}_j \) when the rest of equation (19) has its minimum value.
Figure 14: The quotient $\hat{W}_j/\hat{W}_j$ from equation 19 is shown for different distance between two photon interactions within the tungsten cylinder as a function of photon energy.

Figure 14 shows that $\hat{W}_{j+1} > \hat{W}_j$ is valid for some circumstances within the tungsten cylinder.

There are two different cases when a photon passes the distance $|\vec{r}_j - \vec{r}_{j+1}|$ within two different media in our environment. If the photon goes from tungsten to water, $W_{\text{hom,het}} < 1$. But in the case when the photon goes from water to tungsten, $W_{\text{hom,het}}$ gets its smallest value when the photon path is as much inside the tungsten cylinder as possible thus making the calculations for $W_{\text{hom,het}}$ inside the tungsten cylinder a lower limit.

The results have shown that there were some circumstances that can lead to an increased heterogeneous weight for a photon in the simulation. Increased heterogeneous photon weights contributed to an increase in the scored dose difference $\Delta D^c$ according to equation (11). Values of $\Delta D^c$ which deviated greatly from the average scored value resulted in an increased variance and therefore a decorrelation of the scored values.
5. Discussion

If we consider environments where the heterogeneity is more realistic for a human body, most of the tissues have linear attenuation coefficients comparable to water. In this case the decorrelation between absorbed dose contributions in the homogeneous and heterogeneous environments may be small. Thus we may expect efficiency gain larger than one for regions unaffected by heterogeneities like bones and air cavities. For bones, the linear attenuation coefficient is about 10 times smaller than that of the tungsten alloy used. This makes it more unlikely for the statistical weights to increase as rapidly as in this study case. We may expect a decrease in the efficiency gain but, perhaps, no strong multimodality of the distribution of the efficiency gain estimate. For air cavities, the linear attenuation coefficient is noticeably smaller than that of water. Thus interactions inside the air cavity will decrease the statistical weight of the photon. Again this will lead to a decrease in the efficiency gain and, perhaps, no strong multimodality.

Multimodality of the distribution of the efficiency gain estimate is difficult to predict because it depends on the number of simulated histories. On one hand the central limit theorem says that the usage of a large number of photon histories will lead to a uni-modal, normal distribution. But, on the other hand, it is well known in statistics that the sample variance lacks robustness of efficiency [7]. It means that an efficiency gain estimate defined as a ratio of two sample variances is sensitive to outliers. In the present report and in [2], the sensitivity to outliers was tackled with batching; the batch averages were supposed to be more normally
distributed than individual per-history scores. Our results confirmed that 4 000 samples per batch were not enough to eliminate the effect of per-history outliers. A very different approach was tested in [6]: the bootstrap method was used to estimate the PDF (probability density function) of the efficiency gain estimate. Despite extremely large samples in the bootstrap method (each sample contained $10^8$ values), the multimodality was still present.

One way to resolve the problem with photons with high statistical weights could be to split these photons into several photons with the same sum of weights as the initial photon [6]. This solution would make the calculations more statistically reliable. The splitting of photons will also result in a more detailed and time consuming simulation in areas with high attenuation coefficient, which aren’t always the areas of interest. This could be resolved by using Russian roulette, eliminating some of the photons with high statistical weight in areas which are not of interest.

Though results presented here and in [6] confirmed the high sensitivity of the efficiency gain estimate to outliers, of importance in routine clinical practice is the calculated absorbed dose and its uncertainty; not the efficiency gain of the computational method. The reason why the calculation of absorbed dose uncertainty is not mentioned in this report is that this issue is currently being investigated by prof. Williamson and his team in a separate research project.
6. Conclusion

The purpose of this report was to explain why PDFs (probability density functions) of the efficiency gain estimator had an unexpected multimodal behavior for some voxels and where the problem originated from. It was also of interest to investigate low efficiency gain values. Both the causes and possible solutions of these problems were found as described below.

The unexpected behavior of the efficiency gain estimator was traced back to several histories in the fixed-collision correlated sampling run. These histories had an energy deposit that deviated greatly from the average energy deposit in a batch. It resulted in large values of the scored absorbed dose difference between the homogeneous and heterogeneous environments. (This quantity is used to calculate the absorbed dose in the heterogeneous environment in correlated sampling Monte Carlo methods.) Batch averages containing these outliers were also unusually high and lead to multimodal PDFs of both (i) the estimate of the dose difference variance and (ii) the estimator of the efficiency gain. After the removal of the histories which had high energy deposits, the PDF of the efficiency gain estimator became uni-modal. This also resulted in higher values of calculated efficiency gain. Although the removal of certain histories was a convenience, as it resulted in uni-modal distributions, the efficiency gain estimator became biased.
It was shown that large contributions to the scored absorbed dose in the correlated sampling run were caused by photons with high statistical weights. These rare events occurred when a photon interacted several times within a material with substantially larger linear attenuation coefficient than water.

The existence of photons with high statistical weights is a consequence of the current implementation of the fixed-collision correlated sampling scheme in PTRAN. It is believed that this problem may be mitigated by adding particle splitting combined with Russian roulette to the existing scheme since particle splitting will keep the statistical weight of photons low and Russian roulette will selectively kill unimportant photons and thus shorten computation time.
7. Future work

It can be of interest to investigate the nature of the problem with multimodal PDFs, namely whether the distributions will become uni-modal when more photon histories are used or whether the heavy tails of the scored dose difference will always lead to unstable multimodal frequency functions of the efficiency gain estimator no matter how many histories are simulated. Another thing worth investigating is if it is possible to include particle splitting combined with Russian roulette in PTRAN to handle the problem with high statistical photon weights.
8. Acknowledgments

This thesis was done at the university of Linköping at IMT (Department of Medical Technology) and IMH (Department of Medical and Health Sciences, Division of Radiological Sciences/Medical radiation physics) with the help of Nitai D Mukhopadhyay (Department of Biostatistics, Virginia Commonwealth University), Andrew J Sampson and Jeffrey F Williamson (Department of Radiation Oncology, Virginia Commonwealth University). Special gratitude to Alexandr Malušek (Department of Radiation Dosimetry, Nuclear Physics Institute AS CR v.v.i.) and Gudrun Alm Carlsson (Division of Radiological Sciences/Medical radiation physics) for their guidance and patience during the of this thesis.
9. Appendix

9.1 $\mu$ and $\mu_{en}$ for the used tungsten alloy

Figure 15: Values of linear attenuation ($\mu$) and energy absorption ($\mu_{en}$) coefficients for the tungsten alloy used. Data taken from NIST [8].

9.2 $\mu$ and $\mu_{en}$ for water

Figure 16: Values of linear attenuation ($\mu$) and energy absorption ($\mu_{en}$) coefficients for water. Data taken from NIST [8].
9.3 Matlab functions

This section describes the three main Matlab functions which were used to execute the equations of this thesis.

As can be seen in table 1, only non-zero contributions are listed in the voxel-specific output file. In order for equation (16) to be used, complete history documentation is needed. The Matlab function used to generate \( x \) and \( y \) is listed below.

```matlab
function outdata=batching(indata)

%number of batches
batches=100000000/4000

%the last history present in indata
histmax=max(indata(:,1));

%CReating the outdata vector
XY=zeros(batches,1);

%i is the pointer in the indata
i=1;
%j is the pointer in the outdata
j=1;
%temp is a temporary sum
temp=0;

%The top level while loop
while i<length(indata) && j<batches
    %checks if the history number that i points at is within the batch pointed on by j. If that is the case, the deposited energy is added to temp and i is added by 1, otherwise i points at a history belonging to the next batch. If that is the case, the average of the present batch is added to the outdata and the batch pointer is added by 1.
    if indata(i,1)<=4000*j
        temp=temp+indata(i,2);
        i=i+1;
    else
        XY(j)=temp/4000;
        temp=0;
        j=j+1;
    end
end

%The simulation time was 2.2h, the outdata is multiplied by the square root of the simulation time according to equation (16)
XY=XY*sqrt(2.2);
outdata=XY;
```
The Matlab function for the variance estimators in equation (17) using resampling is shown below. “tracevect” is a massive matrix containing the positions of all the 3000 sample values from x or y used to calculate each of the 50000 values in $s_x^2$ or $s_y^2$, respectively.

```
function [ trace, outdata]=variance(indata)

%the length of the outdata file is set
var_length=50000;
%The outdata vector is created
var_vect=zeros(var_length,1);
%A matrix that will contain all the random batch numbers chosen for each
%element in the variance vector is created.
tracevect=zeros(3000,50000);

%i is the pointer for the var_vect
i=1;

%The top level while loop
while i<=var_length
    %Calling on the randpick function (described later), gives back 3000
    random values from indata (tempvect) and also the position that they’ve
    been taken from(picked_vect).
    [tempvect, picked_vect]=randpick(indata);
    tracevect(:,i)=picked_vect;
    %n is the pointer in the tempvect
    n=1;
    %Calculates the mean value of tempvect
    mean_value=mean(tempvect);
    %temp is a temporary sum
    temp=0;
    %Second level while loop which calculates equation (17) for tempvect.
    while n<=length(tempvect)
        temp=temp+(tempvect(n)-mean_value)^2;
        n=n+1;
    end
    var_vect(i)=temp/(length(tempvect)-1);
    i=i+1;
end
outdata=var_vect;
trace=tracevect;
```
The “randpick” Matlab function used in the code on previous page. This program was written instead of using the inbuilt “randsample” in order to be able to trace which sample values were chosen from \( x \) or \( y \) for each value of \( s_X^2 \) or \( s_Y^2 \), respectively. This was used to trace high values of \( s_X^2 \) and \( s_Y^2 \), back to \( x \) and \( y \).

function [outdata, random_out] = randpick(indata)
%Number of random batches picked from indata
picks=3000;
tempvect=zeros(picks,1);
%A vector with 3000 values between 1 and 25000 is created, this acts as a
map for which values should be chosen from indata.
rand_vector=ceil(rand(picks,1)*25000);
%i is the pointer in tempvect and rand_vector
i=1;
%A while loop which picks out the 3000 values pointed out by rand_vector
from indata and stores these in tempvect.
while i<=picks
    tempvect(i)=indata(rand_vector(i));
    i=i+1;
end
%Both the choosen values and the map which points at these are given back
from randpick.
outdata=tempvect;
random_out=rand_vector;
10. References


