

## **MONTE CARLO DOSE ALGORITHM**

**Clinical White Paper** 

## ABSTRACT

Conventional dose calculation algorithms, such as Pencil Beam are proven effective for tumors located in homogeneous regions with similar tissue consistency such as the brain. However, these algorithms tend to overestimate the dose distribution in tumors diagnosed in extracranial regions such as in the lung and head and neck regions where large inhomogeneities exist. Due to the inconsistencies seen in current calculation methods for extracranial treatments and the need for more precise radiation delivery, research has led to the creation and integration of improved calculation methods into treatment planning software.



Figure 1: The Monte Carlo (XVMC) Dose Algorithm (right) simulates rotational treatments continuously while Semi Analytical Dose Algorithms (left) show discretization artifacts.

iPlan<sup>®</sup> RT Dose with Monte Carlo from Brainlab has been developed in order to compensate for this under dosage in extracranial calculations and improve radiation treatment planning accuracy for clinical practice.

The advanced dose calculation solution from Brainlab is based on the Monte Carlo (MC) method of modelling the transport of radiation through the beam collimation system and through human tissue. Monte Carlo requires a 3-dimensional CT-scan of the patient's tissue to create an internal model of the patient and to calculate the dose distribution of the radiation emitted by a medical linear accelerator. The present implementation is designed to model photon radiation. It can be used to calculate dose for conformal Multileaf Collimator (MLC) treatments including conformal beam, IMRT, static and dynamic arc and HybridArc<sup>™</sup> treatment modalities. The MLC and patient models are created using interaction parameter tabulations from the National Institute of Standards and Technology (NIST) of the USA and the International Commission on Radiation Units and Measurements (ICRU).

Studies have shown that Monte Carlo is more accurate for arc and dynamic IMRT treatments since the MC algorithm simulates gantry rotations and dynamic leaf movements continuously and not in discrete steps as with other algorithms. For these treatments the Monte Carlo calculation might even be faster than the pencil beam. As an integral part of the iPlan RT Dose software, Monte Carlo is designed to provide additional dose planning choice for the clinical



practice resulting in more informed treatment options especially for extracranial indications. This paper introduces the background to the Monte Carlo Dose algorithm and its integration into Brainlab treatment planning software. It provides an overview of the physical features behind the iPlan RT Dose Monte Carlo (MC) algorithm and allows the reader to understand the behavior of the MC algorithm and how it will be integrated into the clinical environment. For more detailed information about the MC techniques in general and the XVMC algorithm in particular, refer to the publications listed in section *References*.



Figure 2: Schematic representation of two particle history examples within the patient model. Illustrated are photons (yellow), electrons (green) and positrons (red). The red dots represent interactions of the particles with atoms of the tissue.

## INTRODUCTION

New cancer treatment techniques like IGRT and IMRT allow more precise dose deposition in the target volume and an improved control of the normal tissue complications. An accurate dose calculation is essential to assure the quality of the improved techniques. Conventional dose calculation methods, like the pencil beam algorithm, are of high quality in regions with homogeneous tissue, e.g. within the brain. However, for treatments in the head-and-neck or in the thorax regions, i.e. in regions consisting of bone, soft tissue and air cavities, an improved accuracy is required. For example, the pencil beam algorithm is known to overestimate the dose in the target volume for the treatment of small lung tumors. The reason is, the pencil beam algorithm calculates dose by scaling pencil beam dose distribution kernels in water to take the tissue heterogeneities into account, but this method has accuracy limitations in these regions. MC dose calculation algorithms, on the other hand, provide more accurate results especially in heterogeneous regions.

The MC technique is a stochastic method for solving complex equations or integrals numerically. MC techniques are based on pseudo random numbers generated by computer algorithms called random number generators. Pseudo random numbers are not really random; however high quality random number generators provide uniformly distributed and uncorrelated numbers, i.e. they behave like random numbers. In other words, two arbitrarily generated pseudo random numbers are independent from each other.

In radiotherapy MC techniques are applied to solve the transport problem of ionizing radiation within the human body. Here the radiation is decomposed into single quantum particles (photons, electrons, positrons). The motion of these particles through the irradiation device and the human tissue is simulated by taking into account the material properties of the different components of the Linac head and the tissue properties



in each volume element (voxel). The photons, electrons and positrons interact with the electrons of the atomic shells and the electromagnetic field of the atomic nuclei. This can cause ionization events. The corresponding interaction properties are based on quantum physics.

For the Linac head these properties can be calculated using the known atomic composition of the different components, for the patient they can be calculated based on the CT images and the Hounsfield Unit in each voxel. The interaction properties are given as total and differential cross sections. Total cross sections characterize the interaction probabilities of a particle with a given energy in a medium with a definite atomic composition. Differential cross sections characterize the probability distribution functions for the generation of secondary particles with definite secondary particle parameters like energy and scattering angle. The random numbers in a MC simulation are required to sample the specific parameters from these probability distribution functions. For example, the path length of a photon with given energy is sampled from an exponential distribution function based on the linear attenuation coefficients along the straight line from the starting position to the interaction point. The type of the photon interaction (photoelectric absorption, Compton scatter or pair production) is sampled from the total cross sections of these processes. After sampling the secondary particle parameters from the differential cross sections, the secondary particles are simulated in a similar manner. This procedure causes a particle history beginning with an initial particle and many daughter particles in multiple generations. The process stops if the remaining energy falls below some minimum energy (also called cut-off energy) or all particles have left the region of interest. Figure 2 shows two examples of possible particle histories.

The MC simulation of charged particles (electrons and positrons) is more complicated and more time consuming than the simulation of photons because the number of interactions per length unit is much higher. However, the so-called condensed history technique allows the simulation of charged particles in a reasonable time. Using this technique a large number of elastic and semi-elastic interactions is grouped together into one particle step and is modeled as a multiple interaction with continuous energy loss of the electrons and positrons along their paths.

At each charged particle step the amount of absorbed energy is calculated and accumulated in a threedimensional matrix. Later this matrix is transformed into dose by dividing the energy in each voxel by the mass of the voxel. Generally, a huge number of particle histories must be simulated in a MC calculation. Otherwise, the number of energy deposition events per voxel is small. This leads to a large variance of the dose value in each voxel and the dose distribution becomes noisy. The effect of noisy dose distributions can be observed at the iso-dose lines if they appear too jagged. Sometimes it is difficult to distinguish between physical and statistical fluctuations. Therefore it is important to calculate a smooth dose distribution with small statistical variance. This statistical variance per voxel decreases with increasing number of histories  $N_{hist}$  as  $1/\sqrt{N_{hist}}$  , i.e. the statistical variance can be decreased by a factor of 2 if the number of histories is increased by a factor of 4. This behavior contributes to the long calculation times of MC algorithms. In general, MC dose algorithms consist of at least two components. One component is a virtual model of the treatment device. It is used as particle source and provides particle parameter (position, angle, energy, charge) distributions close to reality. The second component takes the particles generated by the first component as input. It models the particle transport through the patient and calculates the dose distribution. It is useful to subdivide the first component, the model of the Linac head, into further subcomponents (see below).

For a more thorough introduction into all issues associated with clinical implementation of Monte Carlobased external beam treatment planning we refer to the review by Reynaert et al (2007) or the AAPM Task Group Report No 105 (2007).

#### X-RAY VOXEL MONTE CARLO (XVMC)

The iPlan RT Dose Monte Carlo algorithm is based on the X-ray Voxel Monte Carlo algorithm developed by Iwan Kawrakow and Matthias Fippel (Kawrakow et al 1996, Fippel et al 1997, Fippel 1999, Fippel et al 1999, Kawrakow and Fippel 2000, Fippel et al 2003, Fippel 2004). The XVMC algorithm consists of 3 main components (see Figure 3).

The first component is used as particle source. It models the upper part of the Linac head (target, primary collimator, flattening filter) and generates photons as well as contaminant electrons from the corresponding distribution. The particles are then transferred to the second component, the model of the collimating system. Depending on the field configuration, the particles are absorbed, scattered or passed through. The surviving particles are transferred to the patient dose computation engine. In this third component the radiation transport through the patient geometry is simulated and the dose distribution is computed. In the following sections the 3 components of XVMC are characterized in more detail.

## THE VIRTUAL ENERGY FLUENCE MODEL

The geometry of the target, the flattening filter and the primary collimator does not change when the field

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Figure 3: The 3 components of XVMC.

shape is changed. Therefore, it can be assumed that the phase space of photons and charged particles above the jaws and the MLC is independent on the field configuration. To model this phase space, a Virtual Energy Fluence Model (VEFM) is employed. With some extensions this model is based on the work by Fippel et al (2003).

It consists of two or three photon sources with twodimensional Gaussian shape and one charged particle (electron) contamination source. The photon sources model 'bremsstrahlung' photons created in the target and Compton photons scattered by the primary collimator and flattening filter materials. For the photon sources various parameters are required. For example, the distances of the sources to the nominal beam focus is either estimated or taken from the technical information provided by Linac vendor. The Gaussian widths (standard deviations) as well as the relative weights of the photon sources are fitted using measured dose distributions in air. Additional horn correction parameters are also fitted from these measurements. They model deviations of the beam profile from an ideal flat profile.

The measurements in air have to be performed by a qualified medical physicist in the clinic using an empty water phantom. It is necessary to measure profiles and in-air output factors (head scatter factors) for a variety of field sizes representing the range of treatment field sizes. The profiles must be measured in different directions and with different distances to the beam focus. It is recommended to use an ionization chamber with built-up cap for the measurements. The cap increases the number of electrons in the chamber with the aim of an improved measurement signal. It also removes electrons coming from the Linac head. The cap should be as small as possible to guarantee a high spatial resolution. Therefore, it should consist of a material with high density, e.g. brass or some similar material. The thickness of the cap is estimated such that the depth of dose maximum is reached.

The measured profiles are normalized using the in-air output factors. In this way they provide absolute dose profiles per monitor unit. Then the data can be used as representation of a photon fluence distribution in air versus field size. On the other hand, based on the model assumptions a theoretical fluence distribution in air can be calculated analytically. By minimizing the deviations between both distributions, the free model parameters can be adjusted. The minimization is performed using a Levenberg-Marquardt algorithm (Press et al 1992).

The VEFM also requires information about the photon energy spectrum as well as the fluence of charged particle contamination at the patient's surface. This information is derived from a measured depth dose curve  $D_{meas}(z)$  in water for the reference field size (field size used for the dose – monitor unit calibration). The curve  $D_{meas}(z)$  is used to minimize the squared difference to a calculated depth dose curve  $D_{calc}(z)$ .

Based on the model assumptions,  $D_{calc}(z)$  is given by:

$$D_{calc}(z) = w_{\gamma} \int_{E_{min}}^{E_{max}} dE \ p(E) \ D_{mono}(E, z) + w_e D_e(z).$$

The set of mono-energetic depth dose curves  $D_{mono}(E,z)$  in water is calculated using Monte Carlo and the geometric beam model parameters derived after fitting the measured profiles in air. The set is calculated for a table of energies reaching from the minimum energy of the spectrum  $E_{\rm min}$  up to an energy that is a little larger than the maximum energy  $E_{\rm max}$ . This allows us to use  $E_{\rm max}$  also as a fitting parameter.

In contrast to the original paper (Fippel et al 2003), we model the energy spectrum p(E) by:

$$p(E) = N\left(1 - e^{-iE}\right)e^{-bE}, \qquad E_{\min} \le E \le E_{\max}$$

This function behaves more comparable to spectra calculated using EGSnrc (Kawrakow 2000) and BEAM (Rogers et al 1995) especially in the low energy region. The free parameters l, b and the normalization factor

N are fitted. For  $E_{\rm min}$  and  $E_{\rm max}$  we usually take fix values, but it is possible to adjust them also, because sometimes the maximum energy of the spectrum can be different from the

nominal photon energy setting in MV. The parameter

 $w_{\gamma}$  is the total weight of all photon sources. It is calculated by  $w_{\gamma} = 1 - w_e$  with  $w_e$  being the weight of the electron contamination source. The parameter  $w_e$  is also fitted using the measured depth dose in

water and the formula on  $D_{calc}(z)$ . It requires the depth dose MC computation of a pure electron contamination source in water  $D_e(z)$ . Because most of the electrons originate in the flattening filter, the location of the electron source is assumed to be the foot plane of the filter. The energy spectrum of the electrons is estimated by an exponential distribution as described by Fippel et al (2003).

## MODELING OF THE COLLIMATING SYSTEM

The components of the collimating system (jaws and MLC) are modeled in different ways. The rectangle given by the positions of both jaw pairs is used to define the sampling space of the initial particles. That means only photons and electrons are generated going through the jaw opening. In other words, the MC algorithm assumes fully blocking jaws. The error of this assumption is estimated to be below 0.5% because of the jaw thickness and the attenuation of the jaw material. Furthermore, the beam is additionally blocked by the MLC leading to further reduction of the photon fluence outside the beam limits. The advantage of this approach is that it saves computation time. The simulation of photon histories being absorbed within the jaw material would just be a waste of computing power and it would not have a significant effect on the calculation accuracy.

The MLC on the other hand can be simulated with two different precision levels selected by the user of iPlan



Figure 4: Different MLC leaf designs (from upper left to lower right): ideal MLC (no leakage radiation), tilted leaves (Siemens), step design (Elekta), tongue and groove design (Varian), Varian Millennium, Brainlab m3. Represented are only 4 leaf pairs per MLC.



RT Dose. In the Monte Carlo Options dialog it is possible to choose between the MLC models "Accuracy optimized" (default setting) and "Speed optimized". Depending on this selection and depending on the type of the MLC, one of the MLC models represented in Figure 4 is used for the Monte Carlo simulation. The model of an ideal MLC (upper left MLC in Figure 4) will be used, if the MLC model "Speed optimized" is selected. This model neglects both, the air gaps between neighbor leaves as well as the corresponding tongue and groove design. On the other hand, the thickness of the MLC, the widths of the leaves, the material of the leaves and the rounded leaf tips (if available) are correctly taken into account with the "Speed optimized" selection. Especially for the Brainlab m3 the computation time can be reduced by factors of 2 to 3 using this selection. The influence of the "Speed optimized" MLC model on the dose accuracy depends on the beam set up. It is expected to be small for conformal beams, but it can be larger for IMRT beams. Therefore it is recommended to use the "Speed optimized" option only for the intermediate planning process. The final dose calculation should be performed with an "Accuracy optimized" model. The "Accuracy optimized" model always takes the correct tongue and groove design depending on the MLC type into account (see Figure 4 for a representation of the different leaf designs).

The algorithm behind these models is entirely based on the work published by Fippel (2004). It is a full MC geometry simulation of the photon transport. It takes into account Compton interactions, pair production events and photoelectric absorptions. Primary and secondary electrons are simulated using the continuous slowing down approximation. In this approach the geometries are defined by virtually placing planes and cylinder surfaces in the 3D space. The planes (and surfaces) define the boundaries between regions of different material. For MLCs, in general the regions consist of a tungsten alloy and air. For these materials photon cross section tables pre-calculated using the computer code XCOM (Berger and Hubbell 1987) as well as electron stopping power and range tables precalculated using the ESTAR software (Berger 1993) are used. The particle ray-tracing algorithm is based on bit masks and bit patterns to identify the region indices. In extension to the original paper, further MLC models have been implemented.

#### THE MC PATIENT DOSE COMPUTATION ENGINE

The MC algorithm to simulate the transport of photons and electrons through human tissue is based on the publications by Kawrakow et al (1996), Fippel (1999), Kawrakow and Fippel (2000). XVMC is a condensed history algorithm with continuous boundary crossing to simulate the transport of secondary and contaminant electrons. It takes into account and simulates delta electrons (free secondary electrons created during electron-electron interactions) as well as 'bremsstrahlung' photons. For the MC photon transport simulations, Compton interactions, pair production events and photoelectric absorptions are considered. Several variance reduction techniques like electron history repetition, multiple photon transport or Russian Roulette speed up the dose computation significantly compared to general-purpose MC codes, e.g. EGSnrc (Kawrakow 2000). The MC particle histories can run in parallel threads, therefore the code fully benefits from the use of multi-processor machines, like the iPlan Workstation Premium with 8 or more CPU cores. Gantry rotations (static and dynamic) are simulated continuously. This feature is a big advantage compared to other algorithms like the pencil beam because they need discrete gantry positions to model the rotation.

The photon cross-sections as well as the electron collision and radiation stopping powers are calculated using a 3D distribution of mass densities. The mass density in each voxel is derived from the CT Hounsfield unit (HU). This requires a precise calibration of the CT scanner providing a HU to mass density mapping function. If the mass density  $\rho$  is known in a specific voxel, the total cross section for e.g. Compton interactions  $\mu_c(\rho, E)$  for a photon with energy E can be calculated by:

$$\mu_{C}(\rho, E) = \frac{\rho}{\rho^{W}} f_{C}(\rho) \mu_{C}^{W}(E).$$

The function  $\mu_c^w(E)$  is the tabulated Compton crosssection in water,  $\rho^w$  is the mass density of water and the function  $f_c(\rho)$  is a fit function based on analyzing ICRU cross section data for body tissues (ICRU 1992). The factorization into a function depending only on  $\rho$ 

and a second function depending only on E is an approximation. However the data of ICRU Report 46 (1992) imply that this approximation is possible for human tissue. Figure 5 shows the Compton cross-section ratio  $f_c(\rho)$  as function of mass density  $\rho$  for all materials from ICRU Report 46.



The line in Figure 5 represents a fit to these data. It is given by:

$$f_{C}(\rho) \approx \begin{cases} 0.99 + 0.01 \rho / \rho^{W}, & \rho \leq \rho^{W} \\ 0.85 + 0.15 \rho^{W} / \rho, & \rho \geq \rho^{W} \end{cases}$$

This fit function is used by XVMC to calculate the Compton cross-section. There are a few materials with deviations between the real cross section ratio and the fit function of up to 1.5%. However, these are materials like gallstone or urinary stones. Furthermore, the correct elemental composition in a given voxel is unknown. Only a HU number is known and different material compositions can lead to the same HU. Therefore, the HU number itself has some uncertainty overlaying in this manner the uncertainty of the fit function. The influence of the HU number uncertainty on Monte Carlo calculated dose distributions has been discussed in the literature (Vanderstraeten et al 2007). Similar fit functions exist to calculate the pair production and photoelectric cross-sections as well as the electron collision and radiation stopping powers.

Their dependencies on the mass density of course differ from  $f_c(\rho)$ .

The function  $f_c(\rho)$  is also used to convert mass densities  $\rho$  into electron densities  $n_e$  or vice versa. The relation is given by:

$$n_e = n_e^W \frac{\rho}{\rho^W} f_C(\rho)$$

with  $n_e^W$  being the electron density of water.



Figure 5: Compton cross-section ratio versus mass density for all materials of ICRU report 46 (crosses). The line represents a fit to these data. This function is used by XVMC to calculate the Compton cross-section.



#### THE MC PARAMETERS

Within iPlan RT Dose software the user has some influence on the MC dose calculation accuracy, the dose calculation time and the dose result type. This can be done using the Monte Carlo Options. Four parameters can be influenced:

- Spatial resolution (in mm),
- Mean variance (in %),
- Dose result type ("Dose to medium" or "Dose to water")
- MLC model ("Accuracy optimized" or "Speed optimized").

#### SPATIAL RESOLUTION

The spatial resolution defines the size of the internal MC dose computation grid. It does not mean however that the final MC grid size is exactly equal to the value of the parameter. The MC voxels are constructed by combining an integer number of pixels from the original CT cube. Therefore the final sizes of the voxels are only approximately equal to the value of the spatial resolution parameter. They can also be different for the 3 spatial directions. Furthermore, they cannot be smaller than the initial pixel sizes. The selection of this parameter has a strong influence on the calculation time. Decreasing this parameter by a factor of 2 can increase the calculations for small tumors should be performed with a spatial resolution of 2 to 3 mm.

#### **MEAN VARIANCE**

The mean variance parameter estimates the number of particles histories needed to achieve this variance per beam in % of the maximum dose of that beam. Because everything here is normalized per beam, the final variance in the PTV can be smaller. For example, if we have 5 overlapping beams in the PTV and each beam is calculated with 2% variance, then the variance in the PTV is about 1.

In the non-overlapping regions it remains 2%. Because of the  $1/\sqrt{N_{hist}}$  law mentioned in the introduction, the

calculation time increases by a factor of 4 if the mean variance is decreased by a factor of 2. The final

#### DOSE RESULT TYPE

calculation should be 1% or smaller.

The iPlan RT Dose application allows the calculation of 2 different dose types. The default setting "Dose to medium" means real energy dose, i.e. the energy absorbed in a small tissue element divided by the mass of the tissue element. "Dose to water", on the other hand, means energy absorbed in a small cavity of water divided by the mass of that cavity, whereas some tissue, e.g. bone, surrounds the cavity (see Figure 6). There is no visible difference between "Dose to medium" and "Dose to water" for most of the human soft tissue types. However, "Dose to water" can be up to 15% larger compared to "Dose to medium" for bony tissues (AAPM 2007). This is because of the high-



Figure 6: The difference between "Dose to medium" and "Dose to water". "Dose to medium" should be calculated if the user is interested in the average dose within the whole voxel. "Dose to water" should be calculated if the user has more interest in the dose within small soft tissue cells surrounded by bone material.

density bone causing a higher fluence of secondary electrons in the water cavity and accordingly causing a higher dose compared to the case of the cavity filled also with bone. Therefore "Dose to water" should be selected if the user wants to know the dose in soft tissue cells within a bony structure (see Figure 6). The relation between "Dose to water"  $D_w$  and "Dose to

medium"  $D_M$  is calculated by:

$$D_W = D_M \left( \frac{S}{\rho} \right)_M^W,$$

with  $(S/\rho)_{M}^{W}$  being the unrestricted electron mass collision stopping power ratio for water to that for the medium averaged over the photon beam spectrum. This ratio is approximately 1.0 for soft tissues with a mass density of ~ 1.0 g/cm<sup>3</sup>. It increases up to ~1.15 for bony tissue with mass density up to 2.0 g/cm<sup>3</sup>.

#### MLC MODEL PRECISION

The MLC model precision can be either "Accuracy optimized" or "Speed optimized". "Accuracy optimized" means, the MLC is modeled with full tongue-and-groove design. It takes into account the air gaps between neighbor leaves. The "Speed optimized" option neglects this effect. It employs a model of an ideal MLC (see section *Modeling of the Collimator System* and Figure 4). Therefore this option shortens the calculation time. The section *Modeling of the Collimator System* contains more detailed information about the MLC modeling.

#### DISCUSSION

The XVMC code as basis of iPlan Monte Carlo has been benchmarked by comparison with the "gold standard" MC algorithms EGSnrc (Kawrakow 2000) and BEAM (Rogers et al 1995). It has also been validated by comparison with measurements (see e.g. Fippel et al. 1997, Fippel et al 1999, Fippel et al 2003). A detailed comparison of XVMC with pencil beam and collapsed cone algorithms using measurements in an inhomogeneous lung phantom has been published by Krieger and Sauer (2005). Dobler et al (2006) have demonstrated the accuracy of XVMC relative to conventional dose algorithms using measurements for extracranial stereotactic radiation therapy of small lung lesions. An experimental verification of the Monte Carlo dose calculation module in iPlan RT Dose presented Künzler et. al. (2009) by testing a variety of single

regular beams and clinical field arrangements in heterogeneous conditions (conformal beam therapy, arc therapy and IMRT including simultaneous integrated boosts). They measured absolute and relative dose distributions with ion chambers and near tissue equivalent radiochromic films. The comparison to calculations has shown that the iPlan MC algorithm leads to accurate dosimetric results under clinical test conditions.

Fragoso et al. (2010) performed a dosimetric verification and clinical evaluation of the MC algorithm in iPlan RT Dose for application in stereotactic body radiation therapy (SBRT) treatment planning. They conclude: "Overall, the iPlan MC algorithm is demonstrated to be an accurate and efficient dose algorithm, incorporating robust tools for MC-based SBRT treatment planning in the routine clinical setting".

In a similar investigation Petoukhova et. Al. (2010) presented verification measurements and a clinical evaluation of the iPlan RT MC dose algorithm for 6 MV photon energy. They demonstrate that the Monte Carlo algorithm in iPlan RT "[...] is able to accurately predict the dose in the presence of inhomogeneities typical for head and neck and thorax regions with reasonable calculation times (5–20 min)".

In a second publication Petoukhova et al. (2011) performed a dosimetric verification of HybridArc using an ArcCHECK diode array. The authors conclude that for different treatment sites, "comparison of the absolute dose distributions measured and calculated in iPlan RT Dose with the MC algorithm at the cylindrical shape of the ArcCHECK diode array for HybridArc plans gives a good agreement even for the 2% dose difference and 2 mm distance to agreement criteria."

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