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Optimization of the computational efficiency of a 3D, collapsed cone dose calculation algorithm for brachytherapy

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Brachytherapy dose calculations based on point kernel superposition using the collapsed cone method have been shown to accurately model the influence from finite dimensions of the patient and effects from heterogeneities including those of high atomic numbers. The collapsed cone method is for brachytherapy applications most effectively implemented through a successive-scattering approach, in which the dose from once and higher order of scattered photons is calculated separately and in successive scatter order. The calculation speed achievable is directly proportional to the number of directions used for point kernel discretization and to the number of voxels in the volume. In this work we investigate how to best divide the total number of directions between the two steps of successive-scattering dose calculations. Results show that the largest fraction of the total number of directions should be utilized in calculating the first-scatter dose. Also shown is how the number of directions required for keeping discretization artifacts at acceptably low levels decreases significantly in multiple-source configurations, as a result of the dose gradients being less steep than those around single sources. Investigating the number of kernel directions required to keep artifacts low enough within the high dose region of an implant (i.e., for dose levels above approximately 5%–10% of the mean central target dose) reveals similar figures for brachytherapy as for external beam applications, where collapsed cone superposition is clinically used. Also shown is that approximating point kernels with their isotropic average leads to small dose differences at low and intermediate energies, implying that the collapsed cone calculations can be done in a single operation common to all sources of the implant at these energies. The current findings show that collapsed cone calculations can be achieved for brachytherapy with the same efficiency as for external beams. This, combined with recent results on gains in efficiency through implementing the algorithm on graphical card parallel hardware indicates that dose can be calculated with account for heterogeneities and finite dimensions within a few seconds for large voxel arrays and is therefore of interest for practical application to treatment planning. © 2008 American Association of Physicists in Medicine. [DOI: [10.1118/1.2889777](https://doi.org/10.1118/1.2889777)]

Key words: brachytherapy, dose calculation, heterogeneities, collapsed cone, Monte Carlo

I. INTRODUCTION

The potential to improve the accuracy of the calculated dose is commonly ignored in brachytherapy treatment planning, despite the fact that three-dimensional (3D) imaging is used for localization and, hence, also provides the necessary geometry data for modern scatter dose calculation algorithms. This is different from external beam therapy, where images have been utilized in defining the particle transport geometry for dose calculations for many years. The common method of dose calculation in brachytherapy following the TG43 formalism¹ consists of a summation of dose distributions predefined in a homogeneous water phantom. Although the formalism assures accuracy and consistency of the data used, the approach neglects effects of shields, heterogeneities and finite patient dimensions (see, e.g., Ref. 2). New sources that emit photons of low and intermediate energies, e.g., ¹⁶⁹Yb (Ref. 3) and miniature x-ray tubes,⁴ are substantially easier to

shield than sources that emit higher energy photons, thereby making possible treatments performed in lightly shielded rooms and using patient-customized shields. A large part of the total dose is contributed by scattered photons, especially at low and intermediate photon energies (~20–150 keV) where the dose due to scattered and primary photons become of similar magnitude already at clinically relevant distances from the source of 1–2 cm. The dose from scattered photons depends on the full 3D geometry and common practice can yield significant errors when conditions for production of scattered photons differ from those in a large water phantom, e.g., for implants close to the patient surface or in the presence of high-Z shields.^{5,6}

Accurate calculation of scatter dose in the general case requires methods capable of integrating dose contributions over 3D geometries. Several methods have been proposed, such as Monte Carlo (MC) simulations,^{7–9} 3D implementa-

FIG. 1. Summary of the brachytherapy dose calculation algorithm: Primary dose, D_{prim} , is derived using analytical one-dimensional ray tracing (I). Due to CPE, the distribution of scatter energy released by primary photons (carried by once scattered photons), $S_{1\text{sc}}$, is proportional to D_{prim} . $S_{1\text{sc}}$ is used together with the point kernel for first scatter and an appropriate transport lattice for collapsed cone derivation of the first-scatter dose, $D_{1\text{sc}}$ (II). Similarly, the distribution of scatter energy released by once-scattered photons (carried by twice-scattered photons), $S_{2\text{sc}}$, is proportional to the first-scatter dose $D_{1\text{sc}}$. $S_{2\text{sc}}$ is used with a point kernel for residual scatter and a lattice of transport lines to derive the residual-scatter dose, D_{rsc} (III). The total dose, D_{tot} , is obtained by summation (IV).

tion of the discrete ordinates method to solve the transport equation analytically,¹⁰ and the collapsed cone kernel superposition algorithm adopted for brachytherapy (CC).^{11,12} The CC approach has been used to model the effects of finite phantom dimensions,¹² heterogeneities including those of high Z materials,¹³ and source data connectivity to dose distributions around clinical sources.¹⁴ The CC algorithm has recently been demonstrated to run very efficiently on main-frame parallel hardware like multicore processors and graphical processor units.¹⁵

The calculation time for CC algorithms on sequential hardware is directly proportional to the number of transport directions chosen for discretizing the scattering kernels. The total number of required transport directions (and, hence, the calculation time) is reduced in brachytherapy applications by the use of a successive-scattering approach¹⁶ that applies a two-step modeling: explicitly considering the first generation of scattered photons using a first-scatter kernel and then approximating all subsequent scatter generations by a residual scatter kernel. The aim of this article is to investigate the dependence of the resulting accuracy as a function of the number of directions used in each step. We also investigate if the reduced dose gradients encountered for multiple-source implants can allow a reduction of the number of transport directions required to achieve a certain accuracy. Furthermore, at low and intermediate source energies we investigate if the close-to isotropic properties of photon scattering enable the corresponding point spread kernels to be approximated as isotropic. Such an approximation could yield a significant speed improvement for low and intermediate energy multiple-source implants since only the primary dose calculation would need to be executed per source, while the scatter-dose calculation could be executed in a single step common to all sources.

II. THEORY

II.A. Collapsed cone superposition for brachytherapy

In superposition/convolution algorithms, the dose is calculated through an initial source ray trace to obtain the energy released by the primary photons, followed by a superposition of precalculated (usually by Monte Carlo simulations) point spread kernels.^{17–19} The initial ray tracing also yields the primary dose distribution directly as the collision kerma from primary photons, since photon energies are low enough to assume charged particle equilibrium (CPE). (The primary dose is the absorbed dose mediated by primary photons whereas the scatter dose is the absorbed dose mediated by subsequent generations of photons. The scatter-dose can be further divided into the first- and the residual-scatter doses, then representing the absorbed doses mediated by once and higher orders of scattered photons, respectively.) This also provides an efficient method for clinical source characterization.¹⁴ The CC approach is a kernel superposition method which has been optimized for speed through discretizing the angular part of the point kernel by collapsing the angular cone binning onto a suitably designed lattice of transport lines.^{11,20,21} By use of a successive-scattering approach,^{12,16} the transport is divided into separate steps for first and residual scatter, respectively, as illustrated in Fig. 1.

II.B. Optimizing the computational efficiency

The lattice of transport lines to cover the calculation volume is defined by the directions used for point kernel discretization. The base for this discretization is the set of conical segments obtained from tessellation of the spherical

FIG. 2. A sample of spherical tessellations and cone axis directions for kernel discretization. The number of directions into which the sphere is tessellated is indicated by M and corresponds to the number of transport directions used in CC calculations.

surface into discrete elements. Figure 2 shows a sample of the tessellations for various resolutions used in this work.

The main calculation time of the brachy-algorithm is spent in the CC steps (II and III in Fig. 1). The number of calculation operations, and hence the calculation time on sequential hardware, t_{CPU} , is proportional to the number of transport directions and the number of voxels,

$$t_{\text{CPU}} \sim M \cdot N^3 = (M_{\text{1sc}} + M_{\text{rsc}}) \cdot N^3, \quad (1)$$

where M is the total number of transport directions, M_{1sc} is the number used for first-scatter dose calculation, M_{rsc} is that for residual scatter, and N^3 is the number of voxels in the three-dimensional calculation grid. It has previously been shown that calculations using the two steps of successive scattering can use a smaller number of total directions for similar levels of kernel discretization artifacts in the end result than what is achievable through calculation of the total scatter dose in a single step.¹² Optimizing computational efficiency, hence, translates into searching the minimum number of total transport directions that result in acceptable approximations in dose from discretization artifacts, and how these directions are best split between the steps for first and residual scatter. In the current work, the calculations are done in homogeneous phantoms but the algorithm considers heterogeneities and finite patient dimensions both in deriving the primary dose, the distribution of released scatter energy, and through kernel-scaling corrections.^{12,13} The calculation time scaling in Eq. (1) is therefore valid for both homogeneous and heterogeneous geometries.

Point kernels are more isotropic at low than at high energies due to the underlying cross sections for photon scattering. This can be used to gain speed, since if the kernels can be approximated as isotropic it eliminates the need for alignment of kernel directions versus the rays from the primary source, allowing the two CC steps to be merged and executed in common for all the sources of an implant. An earlier work¹⁶ has shown that it is not appropriate to approximate 350 keV point kernels as isotropic and this is therefore not investigated in this work. Use of isotropic kernels has

earlier been found appropriate at and below 100 keV for direct, total-scatter dose calculations with a straightforward (i.e., not collapsed cone) superposition algorithm.¹⁶ Residual-scatter kernels at these energies have already in previous work been approximated as isotropic.^{12,13} In this work the possibility of also approximating the first-scatter point kernels as isotropic will be investigated. Problems with the isotropic assumption might arise for kernels in high atomic number materials which show a pronounced forward directed peak stemming from elastically scattered photons. A way around this is to neglect the mainly small angular deflections of Rayleigh scattering and instead consider these photons as primaries and adjusting the attenuation coefficients accordingly (see Ref. 13).

It should be noted that the discussion above concerns the possibility of approximating point kernels as being isotropic and is not related to assuming that the brachytherapy sources emit photons isotropically. The anisotropy of clinical sources is accounted for through the primary dose obtained while characterizing sources prior to patient calculations with detailed, primary-and-scatter separated Monte Carlo simulations.¹⁴

III. METHODS

III.A. Point kernels and transport lattices

For this work we designed 15 different kernel-tessellations and their corresponding transport lattices, thus enabling 225 combinations of the transport directions M_{1sc} and M_{rsc} (see Table I). Point kernel data were generated with an extended version of EGS4 and has been described in an earlier work.¹⁶

III.B. Generation of test cases

Dose distributions for a point source located at the center of a cubic water phantom with outer dimensions 18.2 cm $\times$ 18.2 cm $\times$ 18.2 cm were generated for the photon source energies 28, 60, and 350 keV.

Calculations with the brachy-version of the CC algorithm were performed for the 225 available ways of combining $M_{\text{1sc}} + M_{\text{rsc}}$ using a voxel size of 0.2 cm $\times$ 0.2 cm $\times$ 0.2 cm. Isotropic kernels for residual scatter were used in the second CC step for the 28 and 60 keV sources. Calculations were also performed using isotropic point kernels in both steps for a selected number of $M_{\text{1sc}} + M_{\text{rsc}}$ combinations at 28 and 60 keV.

Reference dose distributions to test the different CC calculations were derived using EGS4 Monte Carlo simulations. The Monte Carlo results were fitted to polynomials as a function of radial distance from the source. To eliminate the influence of statistical noise on the results, the polynomials were then used to derive dose values at the midpoints of the cubic voxels used in the CC calculation grid. These distributions will in the following be referred to as “denoised MC.”

Point source dose distributions were superposed to form the line, area, and volume implants as schematically shown in Fig. 3. Equal source strength was used for all positions.

TABLE I. The total number of discrete directions used for the 225 different combinations of the 15 basic kernel tessellations used in this work. For multiple-source configurations (line, area, and volume implants of Fig. 3) the investigation is restricted to combinations with 300 or fewer number of total directions (italic).

M_{rsc}	M_{1sc}														
	20	32	60	72	80	128	180	200	240	320	500	720	980	1280	1620
20	40	52	80	92	100	148	200	220	260	340	520	740	1000	1300	1640
32	52	64	92	104	112	160	212	232	272	352	532	752	1012	1312	1652
60	80	92	120	132	140	188	240	260	300	380	560	780	1040	1340	1680
72	92	104	132	144	152	200	252	272	312	392	572	792	1052	1352	1692
80	100	112	140	152	160	208	260	280	320	400	580	800	1060	1360	1700
128	148	160	188	200	208	256	308	328	368	448	628	848	1108	1408	1748
180	200	212	240	252	260	308	360	380	420	500	680	900	1160	1460	1800
200	220	232	260	272	280	328	380	400	440	520	700	920	1180	1480	1820
240	260	272	300	312	320	368	420	440	480	560	740	960	1220	1520	1860
320	340	352	380	392	400	448	500	520	560	640	820	1040	1300	1600	1940
500	520	532	560	572	580	628	680	700	740	820	1000	1220	1480	1780	2120
720	740	752	780	792	800	848	900	920	960	1040	1220	1440	1700	2000	2340
980	1000	1012	1040	1052	1060	1108	1160	1180	1220	1300	1480	1700	1960	2260	2600
1280	1300	1312	1340	1352	1360	1408	1460	1480	1520	1600	1780	2000	2260	2560	2900
1620	1640	1652	1680	1692	1700	1748	1800	1820	1860	1940	2120	2340	2600	2900	3240

The design of the implants was made having clinical reality in mind, where the volume implant was designed to mimic a prostate implant. For the line implants a denser source spacing (0.2 cm) was used along the source channels whereas the spacing in between the channels of the area implant was 1 cm. The volume implant was cubic and consisted of 125 sources equally spaced by 0.6 cm in each direction.

III.C. Evaluation of test cases

To evaluate the quality of the CC dose distributions as a function of the number of used transport directions, we derived distributions of the relative local dose difference versus denoised MC. The relative local dose difference is defined as

$$\delta D(x_i, y_i, z_i) = \frac{D_{\text{CC}}(x_i, y_i, z_i) - D_{\text{denoised MC}}(x_i, y_i, z_i)}{D_{\text{denoised MC}}(x_i, y_i, z_i)}, \quad (2)$$

where $\delta D(x_i, y_i, z_i)$ is the relative dose difference at voxel (x_i, y_i, z_i) , and D_{CC} and $D_{\text{denoised MC}}$ are the dose values in the CC (evaluated) and denoised MC (reference) dose distributions, respectively. The mean local relative dose difference and its standard deviation were also calculated.

FIG. 3. Schematic view (i.e., not to scale) of the point, line, area, and volume implants. The size of the cubic water phantom is 18.2 cm × 18.2 cm × 18.2 cm. The line implant consists of 17 sources spaced by 0.2 cm, the area implant consists of 5 such lines with a distance of 1 cm in between each, while the volume implant is cubic and consists of 125 sources equally spaced by 0.6 cm in each direction. Sources within each implant are given an equal strength in all calculations.

IV. RESULTS AND DISCUSSION

The variation in mean local relative dose difference and its standard deviation as a function of the total number of CC transport directions for point sources at the three investigated energies are summarized in Fig. 4. The results are based on evaluating CC against denoised MC in the most central 6 cm × 6 cm × 6 cm part of the phantom and excluding use of the sparsest grids (i.e., 20 and 32 directions). As can be seen, mean local relative dose differences are always small, implying essentially that the CC discretization conserves energy. Standard deviations are, on the other hand, higher and mostly dependent upon the number of transport directions used in calculating the first-scatter dose (cf. the close to horizontal lines connecting results obtained with constant number of directions used in the first-scatter step). Thus, a higher fraction of the total number of directions should be utilized during the first-scatter step than during the residual-scatter step. The need for more directions for first-scatter stems from the very steep distribution of energy released by primary photons around a single source that makes CC discretization artifacts with origin in the hottest voxels close to the source manifested at a distance. The need for a dense transport grid is significantly relaxed for the residual-scatter step since the distribution of energy released utilized for kernel superposition in this step is proportional to the first-scatter dose (see Fig. 1) and, hence, is much less steep. The somewhat higher standard deviations seen at 28 keV depend most probably on the even steeper distribution of energy released by primary photons at this low energy due to the higher attenuation coefficient. Figure 4 provides no information on the spatial distribution of the local relative differences but it is important to emphasize that the largest values appear at large distances from the source, i.e., in regions of low doses, since the collapsed cone approach does not yield any discretization

FIG. 4. The mean local relative dose-difference ($\overline{lre}$) between CC and denoised MC and its standard deviation (σ) as function of the total number of CC transport directions for single sources at the three investigated energies. Results on standard deviations obtained at a constant number of CC directions for first scatter are connected with lines and marked with the corresponding number of directions used in the first step (M_{1sc}).

artifacts until cone opening angles exceed the size of Cartesian voxels, see Fig. 7 below and Fig. 4 in Ref. 12.

The need for many directions for CC scatter dose calculations is relaxed as soon as there are several sources present; multiple-source implants yield substantially smaller standard deviations than do single sources for a similar number of transport directions. Similar to that for single sources, the CC

FIG. 5. The standard deviation of the mean local relative dose difference between CC and denoised MC as a function of the total number of CC transport directions for the line, area and volume implants at 350 keV. Results obtained at a constant number of CC directions for first scatter are connected with lines and marked with the corresponding number of directions used in the first step (M_{1sc}). Results obtained at 28 keV and 60 keV are similar.

performance for implants depends mostly upon the number of directions used for first-scatter dose calculations. Figure 5 shows the standard deviation of the mean local relative dose difference for the line, area, and volume implants of Fig. 3, as a function of the total number of CC transport directions, obtained in evaluating CC against denoised MC in the central 6 cm × 6 cm × 6 cm part of the phantom. The total number of directions is restricted to 300 and results are shown at 350 keV. Figure 5 incorporates results from using the sparsest tessellations (20 and 32) for the area and volume implants, but excludes use of these for the line implant. For the area and volume implants, use of 60 directions or more for first scatter is enough to reach standard deviations below 1% while the line source requires approximately three times that amount to reach similar levels. Results at 28 and 60 keV are similar to those at 350 keV. Somewhat higher standard deviations are obtained at 28 keV and a slightly higher dependence on the number of directions used for residual scatter is noted at 60 keV. In Figs. 4 and 5, we compare standard deviations in local dose differences for the various implants in a similarly sized volume, even though the fraction of voxels receiving high doses varies with the extent of the implant. Criteria for accepting results of a dose calculation algorithm depend on whether the investigation is performed in a high- or a low-dose region; see, e.g., Ref. 22. A more relevant way to evaluate the implants would be to choose differently sized volumes that include the implant and extend out to a certain level of dose with respect to, e.g., the mean central dose.²³ Below, we will proceed with presenting such an investigation, choosing the volume implant as an example.

Results of CC using in total 52, 92, and 200 directions and denoised MC cannot be distinguished within and around the volume implant in regions with doses above 5%–10% of the mean central target dose (see the left panel of Fig. 6). Not

FIG. 6. Isodose distributions (left) around the volume implant, as derived from denoised MC and CC using in the latter case a total of 52, 92, and 200 transport directions, respectively. To the right are dose profiles along the center arrow overlayed on the isodose plots. Overlayed on the isodose distributions are boxes indicating regions of high and low doses. The boxes indicate areas of $6\text{ cm} \times 6\text{ cm}$ and $3.8\text{ cm} \times 3.8\text{ cm}$, respectively and the corresponding regions are also marked on the dose profiles to the right. D/R means absorbed dose per radial energy emitted in one decay.

until at a distance of around 5–6 cm from the implant center, where dose values are just a few percent of the mean central target dose, small fluctuations become visible at 60 keV using 52 directions. Linear dose profiles through the implant are inserted in the right panel to indicate the transition from regions of high to regions of low doses. The 52 directions (32 for first and 20 for residual scatter) were chosen to investigate since it corresponds to the lowest number possible using the currently available kernel tessellations (Table I) without repeated use of the same grid for the two steps. The 92 and 200 directions were chosen as to investigate effects of approximately doubling the total number of directions and were split up utilizing 60 and 128 for first- and 32 and 72 for residual scatter, respectively.

Relative local dose differences increase with increasing distance from the implant as shown in Fig. 7 by the maps comparing CC (with a total of 52, 92, and 200 transport directions) and denoised MC. Mean differences (given below

FIG. 7. Local dose-difference maps between CC using 52, 92, and 200 total directions and denoised MC for the volume implant at the three investigated energies. Also shown are the mean and standard deviation of the relative local dose difference in the corresponding $6\text{ cm} \times 6\text{ cm} \times 6\text{ cm}$ most central part of the calculation phantom.

each map) are in all cases less than 1% while standard deviations decrease with increasing number of directions from around 2% down to below 1%.

Demands for accuracy are highest for the part of the volume receiving the highest doses. Figure 8 compares dose volume histograms for the target of the volume implant (the most central $3.8\text{ cm} \times 3.8\text{ cm} \times 3.8\text{ cm}$ cube—outlined as the smallest square in Fig. 6) obtained using CC with 52, 92, and 200 directions and denoised MC. Differences are hardly observable and would not yield any significant differences in parameters of interest in evaluating and reporting treatments such as, e.g., the mean central target dose, the volume receiving 200% or more than the prescription dose (V_{200}), and the homogeneity index or the dose covering 90% of the target (D_{90}).²³

A timing study, based on the results of this work in comparison with a prerelease version of Oncentra Masterplan version 3.0, was performed. It revealed a calculation time of 20 s using 52 CC directions for calculating dose to $86 \times 86 \times 86 = 63\,6056$ voxels on an Intel xeon 3.6 GHz computer, i.e., a speed of 31 800 voxels per second. In comparison, a test implementation on parallel hardware¹⁵ showed a further possible increase in speed by a factor close to 100, i.e., less than a second for $86 \times 86 \times 86$ voxels. This is significantly faster than recently published calculation times for accelerated Monte Carlo simulations of low-energy seed prostate implants.^{8,24}

FIG. 8. Dose volume histograms for the “target” of the volume implant (i.e., the innermost $3.8 \text{ cm} \times 3.8 \text{ cm} \times 3.8 \text{ cm}$ cube which equals the implanted volume plus a 6 mm margin), comparing CC using 52, 92, and 200 total directions and denoised MC, at the three investigated energies.

There is no visible difference in comparing isodose distributions or dose volume histograms for the volume implant as computed by denoised MC, CC with isotropic point kernels for both first and residual scatter and CC with isotropic point kernels only in the residual scatter step at 28 and 60 keV (see Fig. 9). This indicates that it is appropriate to use isotropic first-scatter kernels for these low energy sources. After an individual raytrace for primary dose for each source in an implant, the two CC steps (see Fig. 1) can then be done in a single operation common to all sources. However, photon scattering at 350 keV is too forward directed to utilize the isotropic scatter approximation.¹⁶

V. CONCLUSIONS

The number of transport directions required to keep CC discretization artifacts low decreases significantly in multiple-source configurations where dose gradients are less

steep than around single sources. A total of 50–100 directions are enough to get mean local relative dose differences below 1% and its standard deviation below 2% in regions within and around implants with doses above 5%–10% of the mean central target dose. The total number of transport directions is proportional to the algorithm’s calculation speed, and the number needed for high accuracy around multiple-source brachytherapy implants is similar to that used in clinical applications of external beam collapsed cone calculations. The nearly isotropic properties of photon scattering at low and intermediate energies allow the use of isotropic point kernels with few approximations, which results in the CC part of a dose calculation can be done only once for all sources in an implant at these energies, thereby increasing computational efficiency. Combined with recent findings about improved efficiency through implementing the CC algorithm on parallel hardware, this makes possible 3D dose calculations for large voxel arrays within a few seconds. This is of interest for practical treatment planning applications, since the brachytherapy CC algorithm has previously been shown to be capable of modeling clinical sources, finite patient dimensions, and heterogeneities including shields of high atomic number.

FIG. 9. Isodose distributions and target dose-volume histograms for the volume implant, comparing CC with and without use of isotropic point kernels for first scatter at 28 and 60 keV and denoised MC.

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