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A tool for precise calculation of organ doses in voxelised geometries using GAMOS/Geant4 with a graphical user interface

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Abstract

Introduction: The limit of the method of calculating organ doses using voxelised phantoms with a Monte Carlo simulation code is that dose calculation errors in the boundaries of the organs are especially relevant for thin, small or complex geometries. In this report, we describe a tool that helps overcome this problem, accurately calculating organ doses by applying the "parallel geometry" utility feature of Geant4 through the GAMOS framework.
Methods and methods: We have tried to simplify the use of this tool by automatically processing the different DICOM image modalities (CT, PT, ST, NM), and by including the automatic conversion of the structures found in a DICOM RTSTRUCT file into Geant4 volumes that build the parallel geometry. For Nuclear Medicine applications, the DICOM PT, ST or NM images are converted into probabilities of generation of primary particles in each voxel, and the DICOM CT images into materials and material densities. For radiotherapy treatments, the DICOM RTPlan or RTIonPlan may also be used, hence the user only needs to describe the accelerator geometry. We also provide a Graphical User Interface for ease of use by for inexperienced users in Monte Carlo.
Results: We have tested the functionality of the tool with an I-131 thyroid cancer treatment, and obtained the expected energy deposition and dose differences, given that the particle source, geometry and structures are defined.
Conclusions: In summary, we provide an easy-to-use tool to calculate, with high accuracy, organ doses, taking into account their exact geometry as painted by the medical personnel on a voxelised phantom.

Key words: organ dose; voxel phantom; Geant4; GAMOS; parallel geometry.

Introduction

Ionizing radiation has been beneficially applied in medical imaging as well as in cancer treatment. However, concerns about the negative effects of ionizing radiation present a challenge for accurate dose calculation in Radiotherapy and Nuclear Medicine. The first dose calculations were performed using basic geometries to describe the different organs. But since the emergence of DICOM images, accurate dose calculation has been using voxelised phantoms.[1] This method of dose calculation in each voxel is more accurate than the calculation in simple organ geometries because it integrates the patient's unique characteristics into the calculation.[2] Although voxelised images have long been used in Radiotherapy, there is also an increasing interest in their use in Nuclear Medicine treatements, so as to satisfy the new paradigm of calculating personalized dose, aimed at reducing the risks of radiation cancer caused by treatments or cumulative medical imaging exams.

Although there are many advantages to of using voxel dose calculation, this method still has some limitations. First, the resolution of the CT images is sometimes insufficient, unable to describe very small or thin structures such as skin, blood vessels, skeleton,…[3] Second, the voxelization of an organ or treatment volume may have a negative effect: the edges are no longer smooth but are made up of cubes; therefore, the group of voxels cannot truly represent the geometry of the structure, which results in an inaccurate organ dose calculation.

To describe the organs and treatment volumes, physicians or medical physicists draw contours on each slice of the CT image, building what is called a "structure" in DICOM nomenclature. To estimate the dose in a structure, the first task

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of a simulation code is to find out which voxels belong to which structure. There are several criteria commonly used to define when a voxel is inside or outside a structure. The most frequent the scientific literature are: i) if more than fifty percent of the voxel volume is inside the structure, that voxel will be included; ii) the position of the voxel's center is considered. If the center of the voxel is inside the structure, the voxel is inside the structure, otherwise it is outside. Both of these criteria always include the full voxel volume inside the structure or the full voxel volume outside it, even if it happens that the boundary of a structure crosses the voxel, in such a way that only a fraction is inside it. If this error occurs, the deposited energy in the whole voxel and the full voxel mass are used when calculating the dose, resulting in a wrong dose calculation at the edges of the structure. This error may have a big impact on small, thin and complex structure geometries, which could prove dangerous if it occurs close to an important organ. The effect may be greater when there is a steep gradient of dose between the voxel fraction that is actually inside the structure and the fraction that is outside, which is often the case in dose calculations in treatment volumes, as the medical personnel aims to optimize the dose in the treatment volumes and minimize the dose outside. When the deposited energy is the magnitude of interest, as in calculations of specific absorbed fraction (SAF), i.e., the fraction of emitted energy from the source organ that is absorbed by the target organ per unit mass of target organ), the inaccuracies are usually much bigger.

To overcome the limitations discussed above, many researches have been conducted, including improving the resolution of tomography[4] and the automatic organ segmentation.[5-7] For organs that are small, thin or geometrically complex, attempts have been made to develop dedicated dose calculation methods. Paula C. G. Antunes et al. proposed a method to make the skin simulation more accurate by assigning to the skin a more suitable thickness and its actual location through division of the selected voxels;[8] however, after some voxels are selected for subdivision, there still remains some cubic shapes which cannot represent the geometric flexibility of the skin. Others have tried to develop a specific voxelised phantom with a precise skin definition of 1.5 mm in width;[9] however, the imposition of a defined thickness for the skin is not flexible enough, and the methodology cannot be easily extended to patient voxelised phantoms. Likewise, calculating the dose for the bone is not an easy task due to the difficulty of accurately and completely defining the bone volume. Chung-Yi Huang developed an algorithm for bone segmentation;[10] in his study, a modified marching cubes algorithm, a 3D reconstruction algorithm, is employed to establish a triangular model. Finally, there are some recent researches[11-13] in mesh-type computational phantoms; however, these types of phantoms are not yet in widespread use and are not expected to be used in the clinical environment in the near future. In summary, the limitation of the Monte Carlo method when calculating organ dose in a voxelised image has not been solved yet.

In this paper, we present a solution for this problem, which uses the "parallel geometry" utility of Geant4[14] (also known as "readout geometry"). This utility allows users to load two (or more) geometries, using one as the real geometry (called mass geometry in Geant4 terminology) and the rest for dose calculation. We have developed a tool under the GAMOS framework[15,16] to simplify the use of this method: the user only has to define the DICOM files to be used, and GAMOS will calculate the energy deposited or dose for each voxel or voxel fraction, as well as provide numbers for the whole organs. We illustrate this method with a case of a thyroid cancer patient: the Nuclear Medicine image is used to define the position of the I-131 isotopes and the calculation is done in three structures painted by the medical personnel. The result calculated by the standard Monte Carlo method is compared with the accurate one provided by GAMOS using parallel geometry.

Material and Methods

To perform dose calculation in a structure, it is first necessary to transform the DICOM CT image into a simulation image containing the material properties for each voxel. This can easily be done using, for instance, the Schneider Hounsfield number to material conversion table.[17] If the user adds the name of the DICOM RTSTRUCT file, GAMOS will locate the voxels that are inside each structure and add this information to the file that contains the voxel material information. The criteria used to identify whether a voxel belongs to a structure is that its center is inside the boundaries of the structure. The dose in a structure is then defined by calculating the sum of the energy deposited in each voxel and dividing it by the sum of the voxel masses.

For precise calculation of the dose in a structure which only takes into account the fraction of a voxel that is inside, it is first necessary to build the parallel geometry containing the structure. This is also automatically performed by the GAMOS utilities, so users simply have to tell where the locations of the DICOM RTSTRUCT and the DICOM CT files are. Optionally, as explained below, the parameters that define the precision used in treating the points of the structure that are coincident and collinear can be set. The user can also limit the structure parallel geometry to a region of space. This feature brings flexibility and convenience to users.

The DICOM RTSTRUCT format describes a structure as contours in each of the DICOM CT image planes. A contour is defined by a set of points arranged in order as they were drawn. Because of the precision of the points drawn by the clinical personnel, two points may be very close to each other but not identical. For these cases, GAMOS allows the user to set a distance limit; should the distance between two consecutive points is be less than this limit, the second point will be omitted.

Structures in the human body are very complex, sometimes including holes and twists. To account for all these possibilities, we have selected the "extruded solids" of Geant4.[18] Then, it is only necessary to convert each structure contour into an extruded solid, defining the number of vertices of the polygon, the vertices' coordinates, and always using two planes, one at the top and the other at bottom of each CT slice. As the parallel geometry will only be used for tracking (to define where the structure boundaries are), the material we assign to it is unimportant; we have selected the "G4_AIR" material. This behavior of parallel geometry helps us to accurately calculate the deposited energy in each organ.

Some structures are formed by two or more contours inside one another. These cases should be built in Geant4, as the subtractions of two or more extruded solids. To identify when a contour is completely inside another, we have developed a robust algorithm. However due to possible precision errors in the drawing, the internal contour may protrude from the external one; but in this case, it is not a problem, because Geant4 subtraction solids accept this type of protrusions.

Another difficult case to be treated is when there are consecutive points that are collinear. A Geant4 extruded solid may be built with these types of points, but a warning message is sent at its construction, because the navigation inside is less efficient. If three points are almost collinear, the user can set a limit for the angle created by the two lines connecting the points (using the points in consecutive order, as given in the DICOM file), so that when this limit is exceeded, the two lines will be considered collinear and the midpoint will be removed.

A set of points belonging to the same contour sometimes creates not one but two or more polygons, with lines connecting them. Creating the extruded geometry in this case may be tricky due to the attached polygons and the very small distance between non-consecutive points. Nevertheless, our robust tool can still handle this difficult case. We illustrate the algorithm that we have developed to treat these cases with the example in **Figure 1**. In this example, the lines connecting 3-4, 5-6 and 13-14 should be removed, otherwise there may be some precision errors when determining the assignment of voxel to structures, even if they do not affect the dose calculations. The method starts with selecting a point on the polygon, for example point 1, then we test whether or not point 1 is on a line created by two consecutive points (e.g 2-3; 3-4; 4-5…), using the same precision parameter that is used for the definition of collinear points. If it is, we cut the polygon at the considered point. The process is repeated until all sub-polygons in the same polygon are identified.

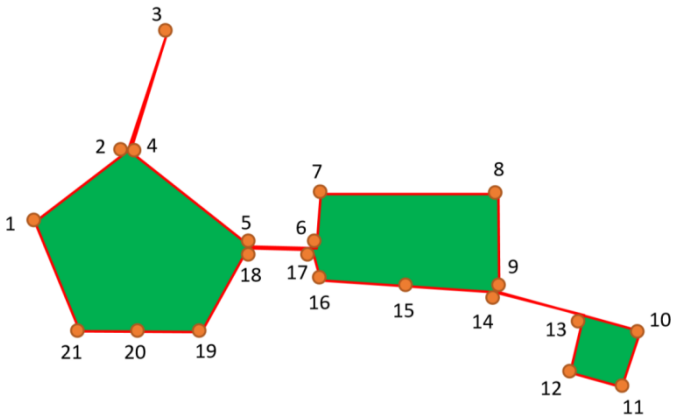


Figure 1. Example of contours joined together

To help the user confirm that the extruded solids accurately reflect the shapes of the structures, we offer a tool that builds for each Z slice an image of the polygon lines of the extruded solids, which are superimposed on the contours of the structure. The user only needs to run a GAMOS example script which receives the geometry containing the extruded solids in Geant4 ASCII geometry format and the DICOM RTSTRUCT file as input. This will print an image file using the GAMOS 2D image printing utility and overlay the image of the structure as defined in the DICOM RTSTRUCT file. By default, the polygon built from the extruded solid is painted in blue, and the one corresponding to the structure is in painted red, and the image limits are adjusted to the minimum covering of the polygons. Nevertheless, the user can also change the colors as well as the image size at will. It is important to note that the GAMOS 2D image utility prints the image based on the volume boundaries as seen by the tracks; this helps avoid the common misconception that the displayed Geant4 geometry is always the same as that seen by the tracks, without taking into account the Geant4 logic for navigation inside overlapping or protruding volumes.

To precisely calculate the deposited energy or the dose limited to the fraction of the voxels that are inside each structure, it is only necessary to add an existing GAMOS filter to the scorer: *GmInParallelVolumeFilter*.

Our tool has been tested by and proven capable of accurately estimating the deposited energy and the dose in several structures for a patient who was undergoing an I-131 thyroid treatment. The thyroid gland is an organ that is neither too small nor too thin, but has a rather complex shape. To assess how the use of the parallel geometry affects dose calculations, we compare the results for each voxel in the defined structures, distinguishing between the voxels that are completely or partially inside them. For the voxels that are partially inside, that is, traversed by the structure boundaries, we examine the dependence among the volume percentage of the voxel inside the structures, the energy and the dose.

Graphical User Interface

Along with the example scripts, GAMOS offers a Graphical User Interface for calculating organ doses. After selecting the directory where GAMOS is installed and the directory where it will be run (where the output files will be written), you can choose the input files:

- Patient description: This can be in DICOM CT format, by selecting the directory where the file set is located or using a file in GAMOS text format, which has been previously created from a set of DICOM CT format files.
- Organs (or Treatment Volumes): The user can select a file in DICOM RTSTRUCT format that contains the structures corresponding to the patient. Alternatively, these structures can be in the GAMOS text file format.
  You may check the box "Calculate Only in Structures", which lies below the button to select structures, if you want the dose to be calculated only in voxels belonging to the same structure.
- Particle source: The first thing to select is the list of isotopes to be simulated. After clicking the "ISOTOPE(S)" button, a new panel will appear, listing 2829 radioactive decaying isotopes, shown in increasing atomic number, and for those with the same atomic number, in order of increasing atomic mass.
  To select where the isotope will initially be placed, there are four options:
  - Use the CT image and distribute the positions evenly across its voxels
  - Use a PET/SPECT image (in DICOM or in GAMOS text format) and distribute the positions proportionally to the activity in each voxel
  - In all loaded structures
  - In a set of structures that is selected from a menu that lists all the loaded structures
- An additional option is to restrict the structures to the fractions of the volumes included in the areas drawn by the medical personnel instead of calculating in full voxels. This calculation uses the algorithm described in this paper.
- The last thing to do is set the number of events, that is, the number of isotopes to be simulated, and click on the "Execute" button.
- Once the calculations are finished, it is possible to visualize them by opening two panels:
  · The first panel shows the list of structures and the dose deposited in each one, as can be seen in **Figure 2**. By default, the simulation doses are given in Gy per initial isotope; it is then possible to set the initial activity of the isotope and the decay time, so that the dose table will appear rescaled. This panel will also display Dose-Volume Histograms for each structure shown. It is also possible to calculate the effective dose if organ conversion factors are provided.
  · The second panel shows the three two-dimensional projections of the CT image, the dose image, or any other image in DICOM or GAMOS text format, as can be seen in **Figure 3**. Currently the GUI is unable to superimpose the dose and CT images, but this will be an upcoming feature. However, since the output dose files are written in DICOM RTDOSE format, they can be viewed with the preferred DICOM image viewer.

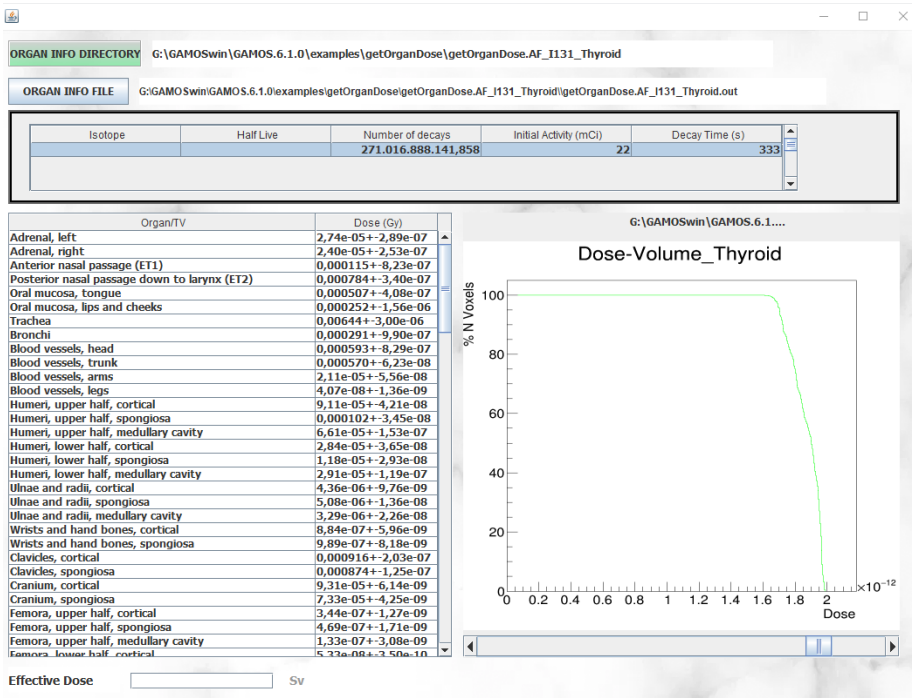


Figure 2. GUI panel displaying calculated dose in each organ and the Dose-Volume histograms

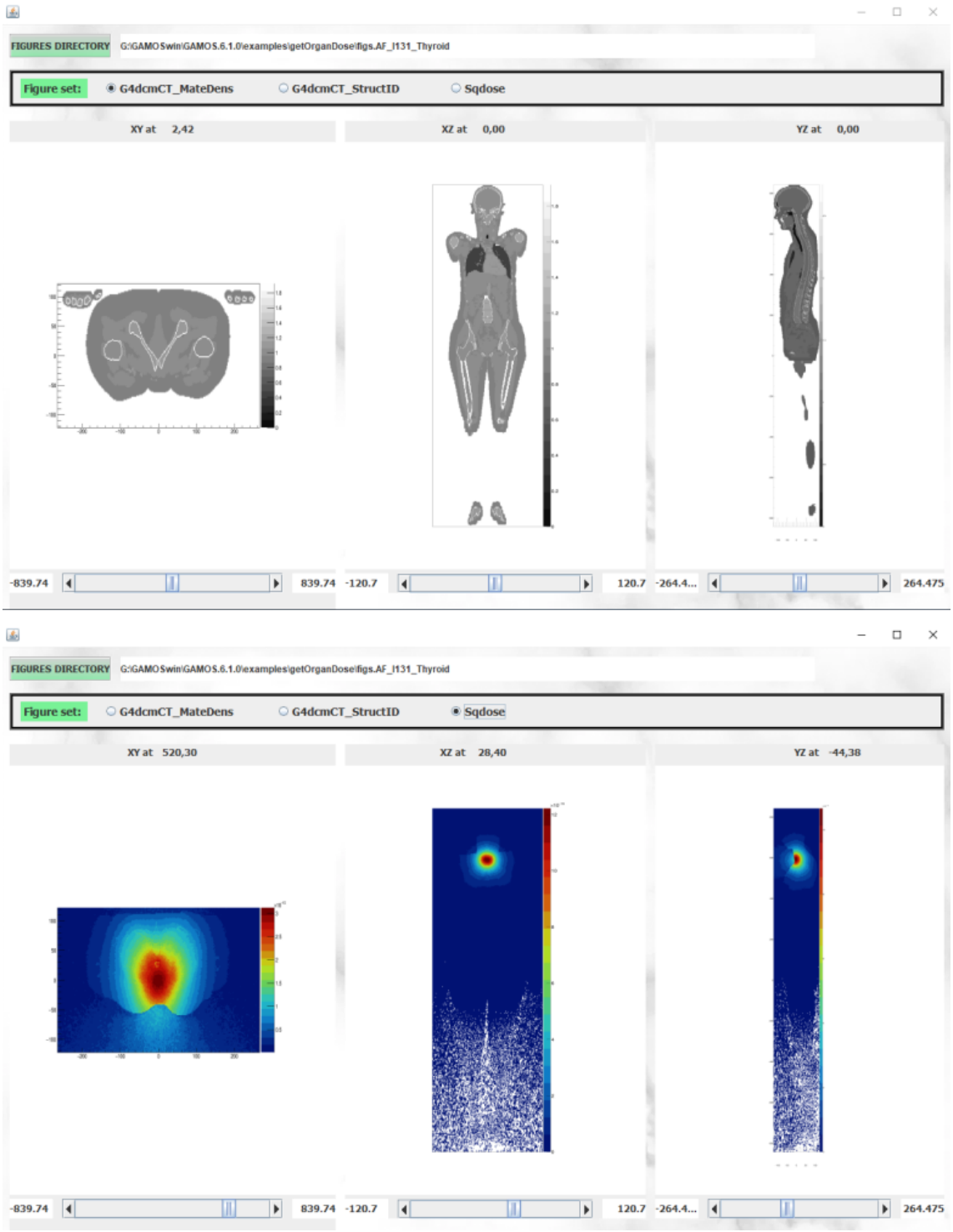


Figure 3. GUI panel displaying the two-dimensional figures of the CT image and the calculated dose image

Results

We have tested our software using a SPECT image of an I-131 thyroid treatment. This DICOM image is used in the simulation as the origin of the isotopes, with the probability of it being placed inside a voxel proportional to the intensity of the image voxel, and the position inside the selected voxel uniformly sampled. The deposited energy and the dose are calculated in the corresponding set of DICOM CT images, using the structures that were defined by the medical personnel and stored in the corresponding DICOM RTSTRUCT file.

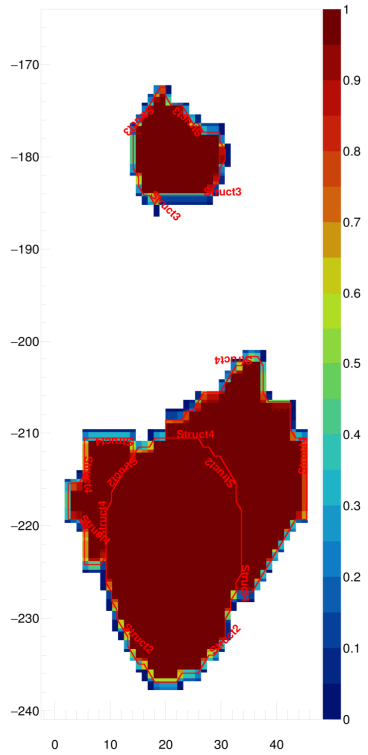


Figure 4. Fraction of voxel volume that is inside the structures for one Z plane. The structures can be seen with their names.

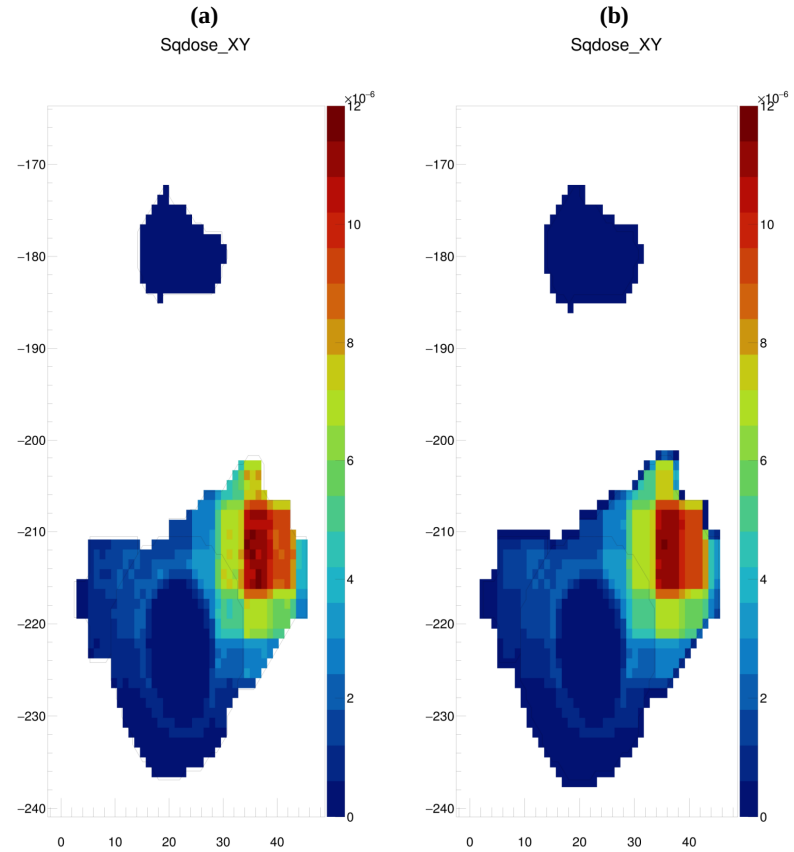


Figure 5. Deposited energy into voxels inside the structures for one Z plane using the standard method (a) and our new method (b).

Figure 4 shows, for one of the XY planes (plane at Z = 1800.5 mm), the fraction of the volume of each voxel that is inside the structures. **Figure 5** shows the deposited energy calculated in the same plane by with the standard method (a) and by with our new method (b). Figure drawing uses the GAMOS DICOM drawing utilities, so color is always applied to full voxels, even though the new method restricts calculations to fractions of them.

To consider the difference between the deposited energy calculated with the two methods, we define a magnitude for each voxel, which we call “Relative Difference”, as the difference between the value of the new method and the value of the old one, divided by the value of the old one. For voxels where the old method value does not exist, we divide by the value obtained from another calculation made without using the structures (that is, deposited energy in each voxel). This Relative Difference is shown in **Figure 6**, with the same plane as the previous figures.

We have checked that for voxels that are completely contained inside the structures, the deposited energy calculated by the standard method coincides with the energy calculated using the old one, making the differences be statistically compatible with zero.

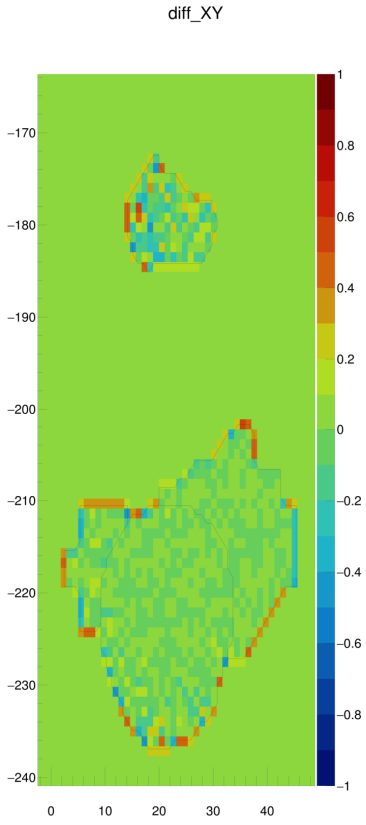


Figure 6. Deposited energy Relative Difference for one Z plane

To better understand the differences in deposited energy, we plot in **Figure 7** the Relative Difference, with its statistical uncertainty (which corresponds to the simulation of 2.e9 isotope decays), versus the percentage of voxel volume that is inside the structures. To better appreciate this figure, we have only repeated it for the five planes with the highest deposited energy. As expected, two diagonal lines can clearly be seen (one for the voxels with centers outside the structures and one for those with centers inside), close to where most voxels are located. We have verified that the voxels that are far from these lines correspond to areas where the deposited energy gradient is larger. We have also visually verified cases in which the lines of the structures cut a voxel with its center outside the structures but with a volume fraction >50% or a voxel with its center inside the structures but with a fraction of volume <50%, finding out that those voxels are cut by two sections of the polygons that limit the structure.

Figure 8 is the same as **Figure 7**, but doses are used instead of deposited energies. In our new method, the voxel volume used to calculate the dose corresponds to the fraction inside the voxel, while the standard method uses the entire voxel volume. As expected, the differences are closer to zero, and only separated from 0 in regions where the dose gradient is bigger.

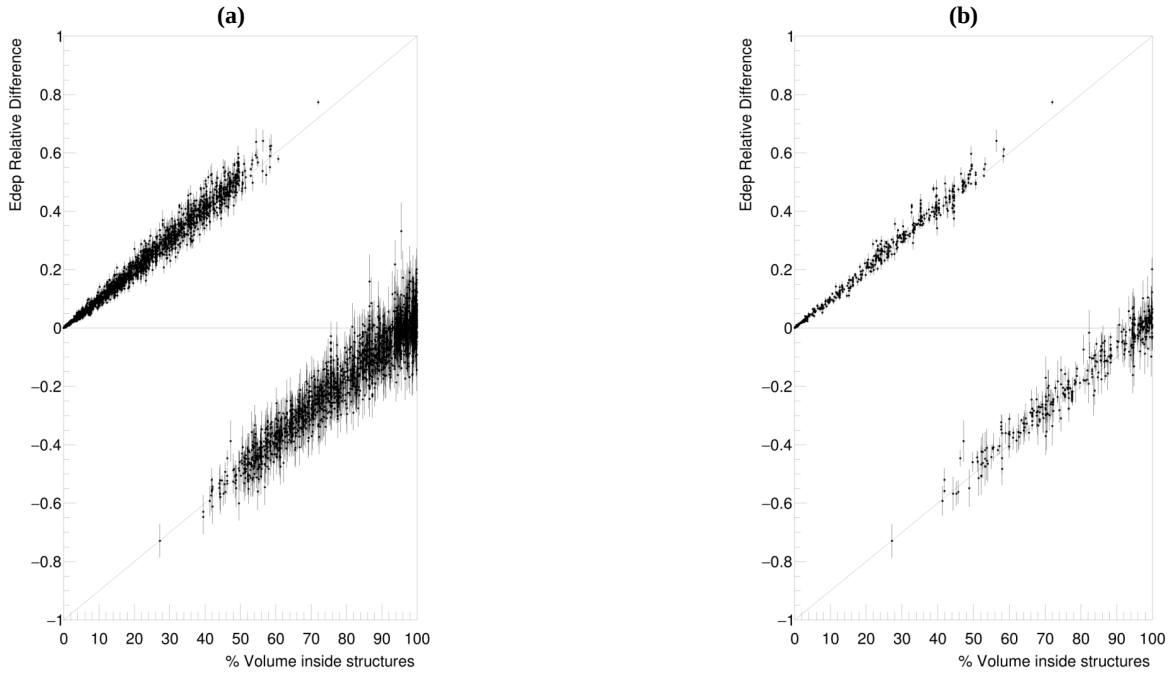


Figure 7. Percentage of voxel volume inside the structures vs. deposited energy Relative Difference, for all Z planes (a) and for only the 5 Z planes with bigger dose (b)

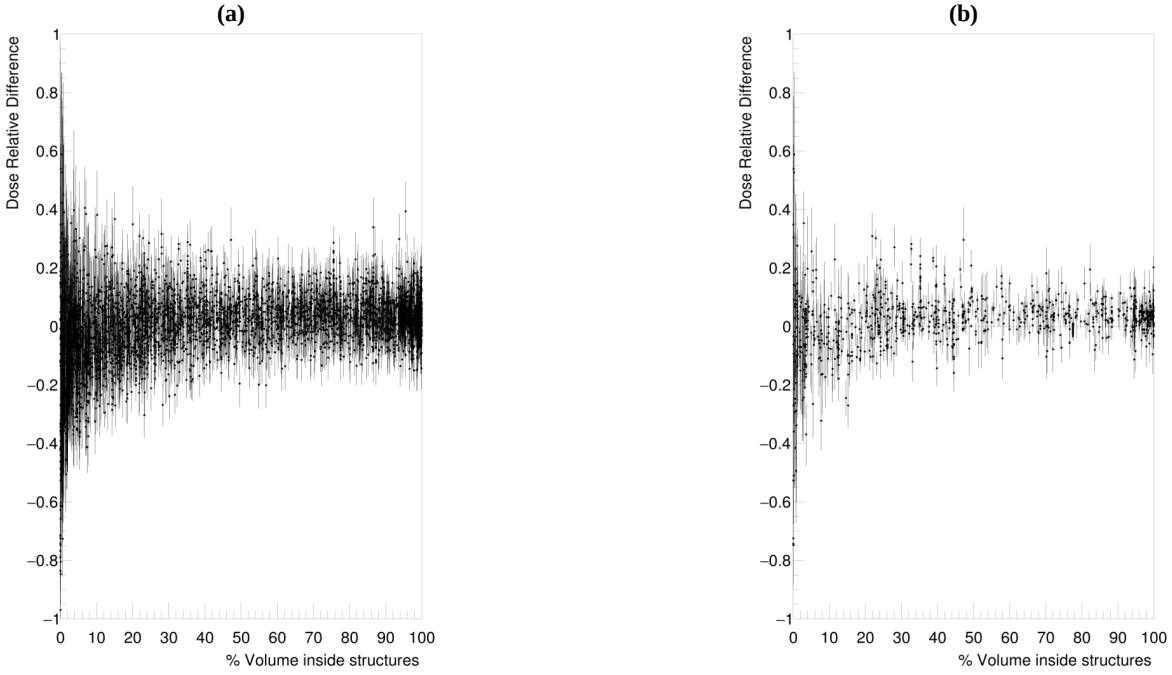


Figure 8. Percentage of voxel volume inside the structures vs. dose Relative Difference, for all Z planes (a) and for only 5 Z planes (b).

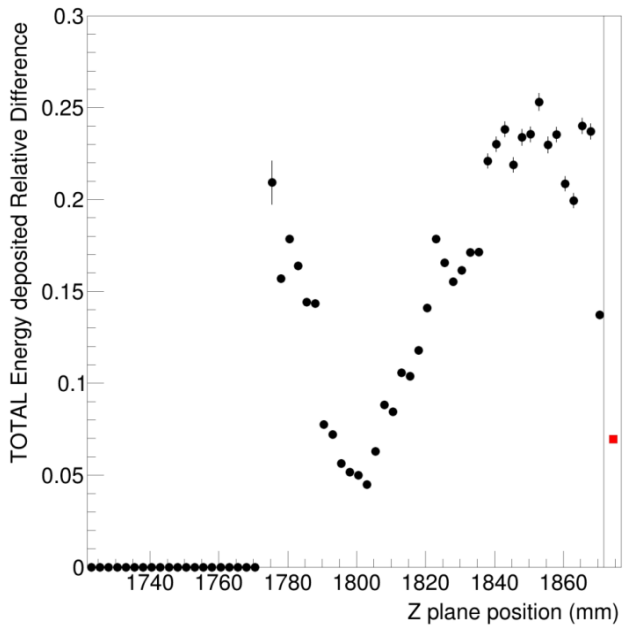


Figure 9. Ratio of the sum of the absolute differences in deposited energy for all voxels in a Z plane and the total deposited energy in that plane, calculated with the standard method, for each Z plane.

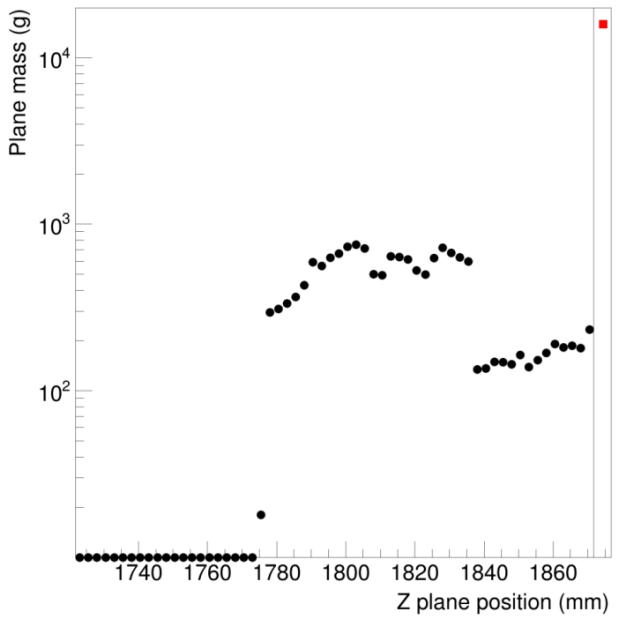


Figure 10. Number of voxels inside the structures for each Z plane

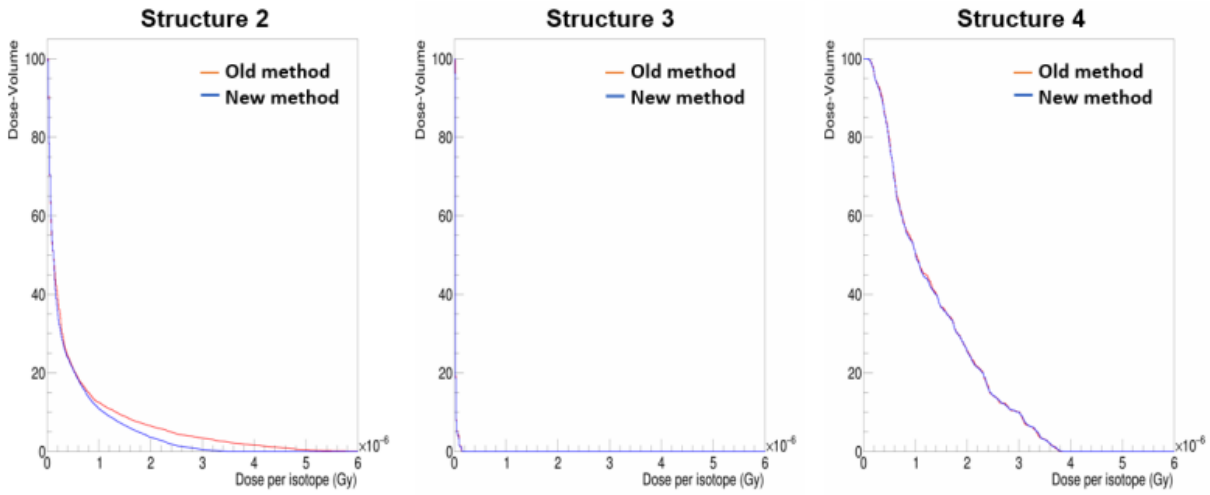


Figure 11. Dose-Volume histograms for each of the three structures comparing the old and the new method.

To summarize the effect of the correction of the new method for the studied configuration, we plot in **Figure 9** the ratio of the sum of the deposited energy differences for all voxels in a Z plane and the total deposited energy in that plane calculated with the standard method. To better quantify this correction, we have added the absolute value of differences of each voxel, since the sum of the differences without absolute value may accidentally result in a value close to zero, which that would not reflect the inaccuracy of the old method. Comparing this figure with the total mass number of voxels inside the structures for each Z plane (**Figure 10**), it can be seen that this correction is a few % for the Z planes with a bigger number of voxels inside the structures, while it can be as high as 25% for the Z planes with a smaller number of voxels (and therefore bigger fraction of volume in the boundaries). Given that for voxels completely inside the structures, the dose does not change when the new method is used and, if we assume a constant density (which is a good approximation in our case), we could estimate from these two figures, that the volume fractions that are receiving an excess or a lack of dose in each Z plane are between 5 and 25 %. **Figure 11** shows the Dose-Volume Histograms, which is common in Radiotherapy. The differences between the standard and the new method are big for one structure, but not as big for the other two. This is actually an expected behavior: the effect of the correction can be large or small depending on the size and shape of the structure and the distribution of energy deposition. In a dose calculation with segmented organs, users do not need to consider which organ needs dose calculation by parallel geometry. If users choose the "Calculate Only in Structures" option, all structures will be converted to parallel geometry and the dose calculated for all structures is the optimal dose, where

the errors at the boundaries caused by the voxelization will be eliminated. A comprehensive assessment of the realistic effect of this new method in different patient cases is beyond the scope of this paper, the main objective of which is to present a free tool for making more accurate organ dose calculations.

Discussion

In this paper we offer a resolution to the inaccuracy of the Monte Carlo calculations in voxelized phantoms of energy or dose deposited in organs or other structures, such as Treatment Volumes, when full voxel volumes are used despite the fact that only a fraction of them are really inside the structure. To eliminate the errors at the boundaries of the structures, we have developed a new feature for GAMOS, which is based on the use of the Geant4 parallel structure mechanism, to accurately calculate the energy deposits inside a structure, restricting calculations to the actual fraction of voxel that is inside it.

We have also developed the tools to facilitate the use of this method in GAMOS. For Nuclear Medicine calculations, the user only has to provide the corresponding DICOM PET/SPECT, CT and RTSTRUCT files, and GAMOS takes care of constructing the parallel geometry, converting the structures into Geant4 extruded solids, replacing the file locations, and calculating the deposited energy or the dose map, which can be dumped into a DICOM RTDOSE file or in a binary file if statistical uncertainties are to be saved. For a radiotherapy treatment, the user only needs to add the linac geometry description or a phase space file as input to the dose calculation. The tool is offered for free with the GAMOS software, with some example scripts that we hope will suit the needs of a wide community. A Graphical User Interface is also available, so calculations can be done simply by clicking on a few buttons.

With the sole objective of testing the software, we have applied the tool to a patient treated with I-131 and obtained the expected differences in deposited energy and dose for each voxel, given the geometry and the distribution of activity. The CPU time increase when the new method is used is only 17% over the standard method time. As expected, the differences between the standard and the new method are bigger for the calculations of deposited energy than for the dose, making the tool especially valuable for studies in which the magnitude of interest is the organ absorbed fraction. However, it should be noted that although the dose in the boundary voxels may not change much with the new method unless there is a big dose gradient, the important figure is the dose-volume, or in other words, for how much volume the dose is erroneously calculated by the standard method, especially if this volume belongs to a nearby organ that is meant to be protected.

Regarding the clinical utility of this tool, it is still something to be proved, and we plan to do a more systematic analysis of Nuclear Medicine and Radiotherapy cases in a future work. This study will also analyze the lack of precision in the rendering of contours by comparing the structures defined by different medical personnel to better understand the utility of this tool. What seems clear so far is that it is a powerful tool if the organ to be analyzed is the skin, or other thin or small organs, where, even if the medical personnel make a very precise drawing of the structures, standard Monte Carlo simulation would not be able to make an accurate calculation.

Conclusions

In summary, we offer a method of accurately calculating deposited energy and dose taking into account only the fraction of each voxel volume that is actually inside the structures painted by the medical personnel, along with tools to simplify how it is used. We believe that this tool will be especially valuable for calculations in thin, small or oddly shaped organs or treatment volumes. Since we also offer a Graphical User Interface, we hope that the tool will also be usable for non-expert software users.

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