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VoxelMages: a general-purpose graphical interface for designing geometries and processing DICOM images for PENELOPE

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ABSTRACT

The design and construction of geometries for Monte Carlo calculations is an error-prone, time-consuming, and complex step in simulations describing particle interactions and transport in the field of medical physics. The software *VoxelMages* has been developed to help the user in this task. It allows to design complex geometries and to process DICOM image files for simulations with the general-purpose Monte Carlo code PENELOPE in an easy and straightforward way. VoxelMages also allows to import DICOM-RT structure contour information as delivered by a treatment planning system. Its main characteristics, usage and performance benchmarking are described in detail.

1. Introduction

Monte Carlo (MC) techniques used in medical physics, and in particular in radiotherapy, constitute a rapidly growing field. In fact, modern cancer treatment considers these kind of calculations as the gold standard to compute the dose distribution in any radiotherapeutic modality. A necessary previous step in any MC study is to design the set-up involving either internal and/or external radiation sources, often a tedious, complex, and error prone work. This is the case of the MC suite PENELOPE (Baró et al., 1995) whose geometries are given in text files, either by parameterizing quadric surfaces, making the use of rotations and translations of the objects cumbersome, or by specifying the mass density and material composition for each point in a discretized volume. For this reason the software *VoxelMages* (Voxelizing and making Geometries for Simulations) has been developed. This software makes the building of these geometries much easier by providing the user with a three-dimensional interactive display during their design. Moreover, this software allows to voxelize the geometry or to import DICOM files generated elsewhere, to process them and to generate a voxel file in the PENELOPE standard format. DICOM-RT structure contours can also be extracted. Once these contours have been imported, *VoxelMages* allows to define material composition based on them. Finally, it allows to start simulations using the software PENELOPE and to visualize the resulting dose distributions using the included 3D viewer.

The program code is open source and available under the GPL license. It has been written in C++ with subroutines in bash. In order to create the graphics it makes use of the OpenGL library (OpenGL Architecture Review Board, 2015). To open and read DICOM files it takes advantage of the dicomsdl library (dicomsdl, 2015). Thus, the only external program needed to compile *VoxelMages* is a C++ compiler, although it is recommended to use the GNU g++, standard in any Linux distribution. Hence, it does not require any proprietary software.

The current version of the program exports the geometry and voxel files in a format compatible only with PENELOPE. However in the future it is planned to add support for other formats and also to implement the possibility to import/export geometries between different MC systems.

2. Materials and methods

2.1. PENELOPE

PENELOPE (Baró et al., 1995) is a state-of-the-art MC code that has become widely used to tackle a wide variety of fields, from microdosimetry to electron microscopy to name a few. A comparison of simulation results with experimental data has been reported elsewhere (Sempau et al., 2003). PENELOPE is a general-purpose code system originally designed to simulate coupled electron-photon transport in arbitrary material systems consisting of a number of homogeneous regions limited by sharp interfaces. It has recently been extended to incorporate the transport of protons (Sterpin et al., 2013). This code allows to simulate materials with arbitrary chemical compositions for electrons and photons with initial energies ranging from a 50 eV up to 1 GeV. The different structures forming a simulation

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are constructed by using either quadric geometries, i.e., two-dimensional surfaces that are the locus of zeros of a quadratic polynomial, or through voxelized geometries, i.e., structures are defined in a Cartesian grid where for each sub-volume (voxel) the density and material are given.

The main advantage of PENELOPE, its generality, may become a drawback since to be operative it must be completed with a steering main program developed by the user. This implies that the user must be proficient in Fortran77 to 95, something that it is not usually the case in clinical practice nowadays. To overcome this, Sempau et al. have developed penEasy (Sempau et al., 2011), a general-purpose main program for PENELOPE. penEasy allows the user to specify a series of source models and tallies from a preprogrammed structured code. In the following, when we refer to the PENELOPE features and capabilities we will be implying the simultaneous use of PENELOPE and penEasy.

2.2. The voxelmages software solution

As mentioned above, *VoxelMages* has been entirely written in C++ and it is being distributed as open source software under the GPL license. This will allow any user to compile the code on his/her own computational facilities. The present version can be run in any Linux-based system. Following the standard determined by PENELOPE, all distances are given in centimeters (cm), all masses in grams (g), and all energies in electron-volts (eV). In Fig. 1 the main program interface is shown. The window on the left provides the user with a side view of the geometry, the top right one provides a view with the camera positioned above the geometry, and finally the lower right window shows a view with the camera situated below the geometry. The different features of the program are described in the following..

2.2.1. Designing quadric geometries

In medical physics, one often needs to perform Monte Carlo calculations including an imaging device, a detector, a brachytherapy seed, etc… That is, any device with well-known blueprints and material composition. To do that, the device geometry can be modeled in PENELOPE using quadric surfaces like planes, cubes, spheres… etc. *VoxelMages* provides the user with a set of tools to ease the construction of such geometry under the section **Geometry construction**.

To create an object the user needs to select the tool *New object*. This option allows the user to build a body using the most common quadratic surfaces included in PENELOPE, i.e. planes, cylinders, cones, spheres, or any combination thereof. In subsequent versions of VoxelMages this list may increase to include the rarely used hyperboloids. In all cases, the coordinates (x, y, z) of the center of the object have to be provided. Six different bodies can be constructed.

- Prism: the length of the lateral sides have to be specified. First, the length of the face parallel to the x axis must be entered, next the same for axis y and z. The center entered into the program is assimilated to the geometric center of the prism.
- Cylinder/cone: to add a cylinder or a Cone the user must enter the height and the radii of the top and bottom basis. The center used by the program is located at half the height of the cylinder/cone.
- Sphere: only the radius of the sphere is needed.
- Sphere section: the user is required to enter the radius of the sphere and the height where the plane that intersects the sphere intersects the z axis, taking as origin the center of the sphere.
- Infinite plane: it does not require any dimension. To ease the visualization, an infinite plane is shown as a full circle.

Once the dimensions and position of each body are specified, the user needs to assign them a number. Such body number also establishes the order in which they will be created, being the one with the lowest value the first to be implemented. In the case of overlapping bodies it should be specified which bodies are embedded (totally or partially) within others. To do so, the number of the internal bodies are added to the list displayed in the outer one. It should be noted that the number of the internal bodies must be higher than those of the external ones, otherwise they would be created before the external one which would superimpose on the former. It should be noted that the body numbers provided by the user might differ from the ones written by *VoxelMages* in the final geometry file because some modifications in the ordering might be required in order to comply with PENELOPE standards.

VoxelMages allows creating a customized body different from these ones. To do so the user will provide all the bodies to be combined with the same body number and *VoxelMages* will create a new body as an intersection of all the given surfaces. Finally, a material number has to be specified to every body in the simulation.

The rotations of the bodies are determined by their Euler's angles. The program uses the same convention as the one followed by PENELOPE, namely, a first rotation around the z axis, a second one about y and, finally, another rotation around the z axis. Nevertheless, the orientation of both the sphere section and the infinite plane are determined by the normal vector of the body plane and hence the user must enter the (x, y, z) components of this vector.

VoxelMages implement several tools to help the user to display and modify the geometry. The *Select object* tool allows the user to delete or modify the parameters of any of the bodies. In order to identify the selected body all the other ones will be displayed translucent. The *Color* option will color the figures depending on their object number, material or body number. A color legend showing the color assigned to the figures will be displayed on the left side of the main window. The user can use the keys “w”, “a”, “s”, and “d” to displace the point of view, “+” and “−” to zoom in or out and the mouse to rotate the view. The *Save* and *Load* tools allow the user to store the current geometry in an internal format and to recover it for subsequent modifications. The *Save* option also may create a text file in a quadric-based format compatible with PENELOPE. *translations* allows to displace a combination of objects, i.e. a brachytherapy seed or an accelerator head. Support for other formats compatible with other simulation systems could be added in future versions of *VoxelMages*.

Although for the sake of clarity a predefined set of axis is shown, it should be noted that the whole geometry will be included, independently of whether it is inside or outside the displayed volume.

2.2.2. DICOM image processing into voxelized geometries

Digital Imaging and Communications in Medicine (DICOM) has become the standard for managing information in medical imaging, and as such it has to be easily imported into any MC code devoted to evaluate realistic clinical cases. PENELOPE does that by introducing the possibility of obtaining the geometry of a system by means of voxelized geometries in a given format in plain text (see (Sempau et al., 2011) and the code documentation for details).

Unfortunately, PENELOPE does not import directly either DICOM files as a geometry or DICOM-RT structure contour information. *VoxelMages* allows importing the slices stored in a DICOM image obtaining a 3D/2D representation by means of the tool *DICOM loader* and the organ contouring, if existing. In the particular case when the DICOM-RT correspond to a brachytherapy treatment, *VoxelMages* will also import the implant plan, i.e. seeds positions and dwell times. From those, any subset of the image can be selected, and then exported into a voxelized geometry file.

The procedure is as follows. First, the user must save all the DICOM images of different slices in a folder. Then, a text file with the name *calibration.txt* that specifies the calibration of the image device, either computed tomography (CT), ultrasound (US), or both must be created. *VoxelMages* detects automatically whether the DICOM image has been created from a CT or a US, and then it will use the information contained in the calibration file accordingly. The parameters required

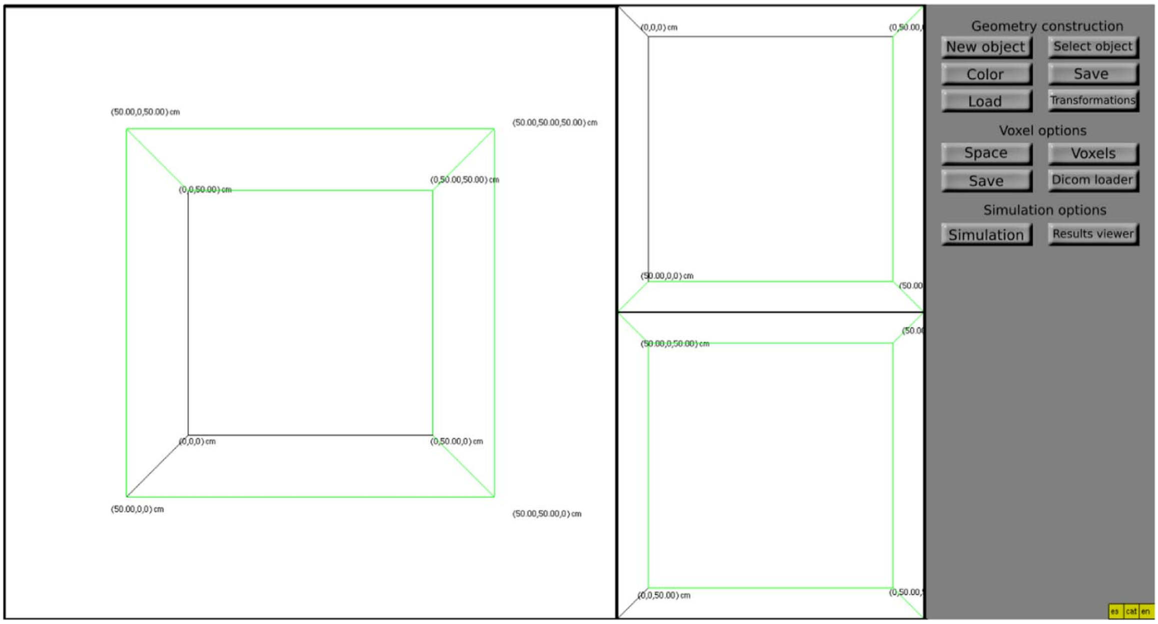

Fig. 1. *VoxelMages* main interface.

Table 1
Example of the required parameters and format to be used in a DICOM calibration file.

CT	US
—Calibration data—	—Contour data—
Number of coefficients=2	Contours number=2
a0=1.01	Target priority=1.0 Density=1.0
a1=8.0e−4	Urethra priority=1.2 Density=1.2
—Materials data—	
Number of materials=2	
Material 1: rho inf=0, rho sup=1	
Material 2: rho inf=1, rho sup=2	

by *VoxelMages* are summarized in Table 1. The headers *calibration* and *material data* will be read only when *VoxelMages* identifies the DICOM file as a CT. This section contains the information necessary to translate the Hundfield units (HU) stored in the DICOM file into the mass density (g/cm^3) values required by the simulation. To do so, *VoxelMages* assumes that the HU calibration is a polynomial of order n with a set of $n+1$ coefficients. The number $n+1$ of such coefficients and their values has to be given. Once the mass density is known, *VoxelMages* assigns the material compositions depending on their values. In this case, the number of different materials and the mass density range for each one has to be specified. Optionally, if the section *materials data* is not present, the program will use as default values those recommended by TG-186 (Beaulieu, 2012). For those DICOM files obtained from a US and containing contouring information, only the header *contour data* will be used. The number of contours, their priorities, and their mass densities have to be provided. The priority will indicate *VoxelMages* which volume is embedded inside each other (outer volumes will have larger priorities than inner ones).

Once the folder containing the DICOM files and the calibration file

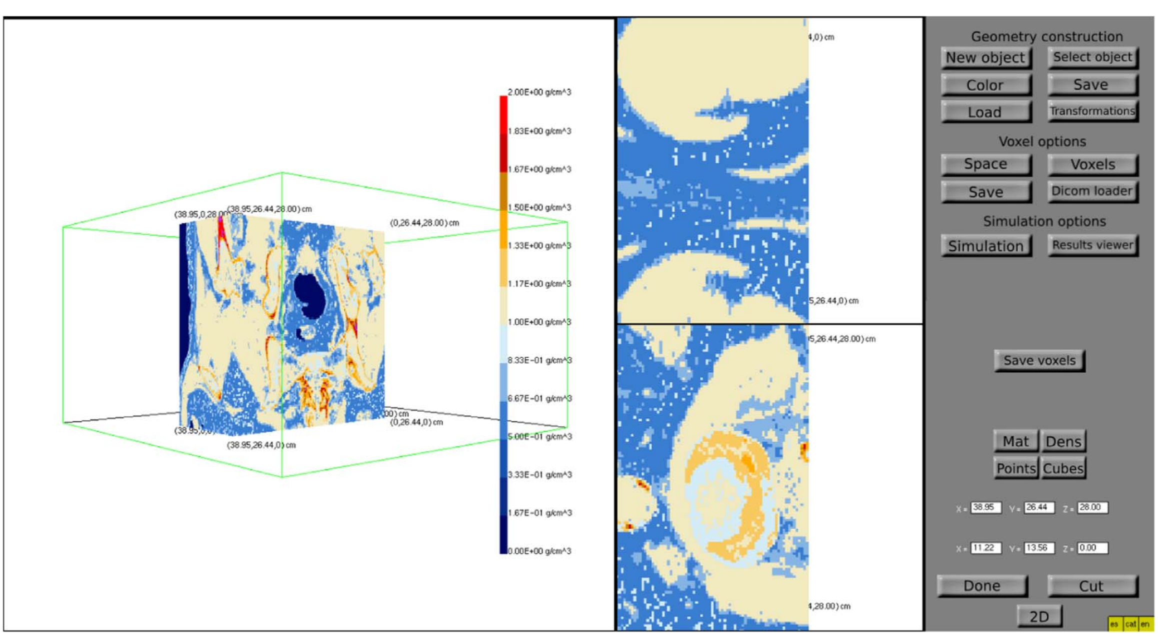

Fig. 2. DICOM image 3D viewer. (For interpretation of the references to color in this figure, the reader is referred to the web version of this article.)

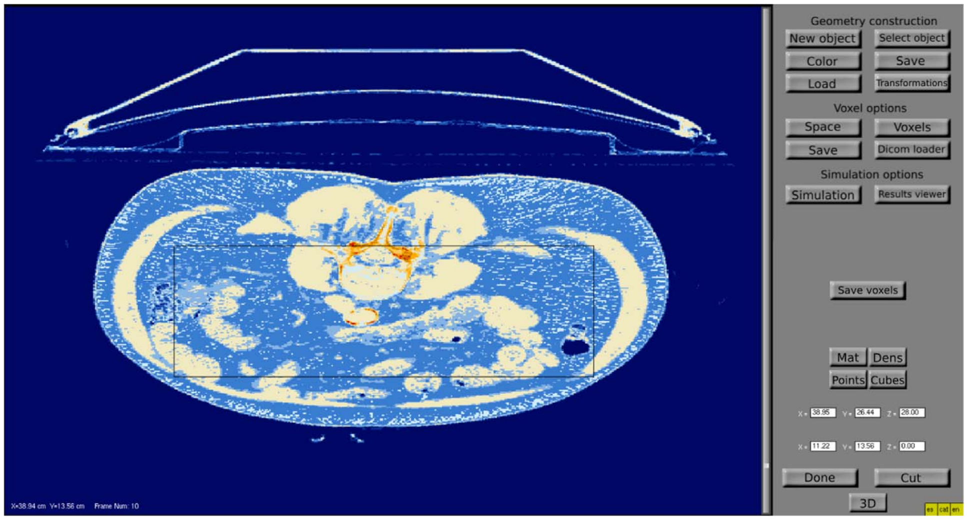

Fig. 3. DICOM image 2D viewer. The black square delimits the selected region before imposing any cut.

has been loaded, the program starts processing and importing all images. When finished, the program creates a 3D view in which the user can switch between the material and density views. To optimize the rendering, the program only draw by default the center point of each voxel. This feature my be changed using the options *Points* and *Cubes*. In addition, the user can select the area of interest for the simulation by entering the lower and upper delimiting planes (x_0, y, z), (x, y_0, z), and (x, y, z_0) and then using the *Cut* option to remove the voxels outside the selected region. Finally, the data from the target area can be exported to a voxelized PENELOPE geometry file. Note that the exported data will contain all the voxels in the cube limited by the axis (green lines), even if those voxels are not visible. An example is shown in Fig. 2..

To simplify the selection task, the user can change into a 2D view where all the slices can be seen individually and the target region can be selected using the mouse. The 2D viewer also includes the possibility of visualizing contours and the material assigned to them. In the case of a brachytherapy treatment the location of all seeds will be displayed. An example is shown in the Fig. 3..

2.2.3. From quadric geometries into voxelized geometries

In some particular simulations it might be useful to create a geometry using quadric geometries and then exporting it in the form of a voxelized geometry. *VoxelMages* implements this feature in the **Voxel Options** section. *Space* permits to change the total volume where the geometry is defined. To modify it, the user is required to enter the new length along each voxel axis and the total number of voxels. Only the bodies inside the total volume will be voxelized. The option *voxels* allows the user to display the voxel representation of the geometry. The color will be assigned depending on its material. To ease the visualization, the material numbered 1 will not be represented in the voxelization. For this reason it is advisable to allocate the material number 1 to the phantom material. Moreover, the user can choose between representing the center point of the voxels, which can significantly boost rendering performance and allows for an easier placement of the camera according to the user needs, or representing the full cubic voxel. In order to voxelize the geometry, the user needs to enter the density of the material. Finally, the voxelizated geometry can be cut by entering the value of the limiting planes. *Save* will create a voxelization of the geometry in a format compliant with the PENELOPE standard.

2.2.4. From DICOM-RT contours into voxelized geometries

Another tool included in *VoxelMages* to create a geometry file is the possibility to export a clinical plan directly into PENELOPE. First, as described in Section 2.2.2, materials can be specified depending on the contours included in a DICOM-RT structure file. Then, *VoxelMages* automatically identifies the different volumes limited by these contours and creates a voxelized geometry including for each voxel the corresponding material and mass density. If brachytherapy seeds are included in the clinical plan, their positions will also be listed in the geometry file so the MC user may take advantage of the mixed geometry feature included in PENELOPE (the possibility of combining quadric and voxelized geometries). In addition to that, *VoxelMages* also generates a text file including all contours data in plain text to be used in any homemade code to evaluate clinical parameters, i.e. dose volume histograms, etc.…

All the visualization options described in Section 2.2.3 also apply here.

2.2.5. Simulation and results viewer

Having constructed a geometry as described in the previous sections, *VoxelMages* implements the possibility to run a MC simulation using the PENELOPE system simply by selecting the option *Simulation*. The user needs to provide: (i) a name for the simulation, (ii) the name of the configuration file, (iii) the name of a geometry file, and iv) the number of simultaneous parallel simulations to run. *VoxelMages* will divide the complete simulation into partial simulations and will run them simultaneously. Once the simulations have finished, the program will combine all the partial results from the subtasks and save the final end result into a single file.

The *Results Viewer* tool allows the user to display a representation of the voxelized dose distribution resulting from any PENELOPE simulation. The user needs to enter the name of the folder which contains the end-result file. The program reads it and represents the dose distribution in linear or logarithmic scales. To ease the visualization, a minimum and a maximum values of the dose to be displayed can be selected.

3. Results and discussion

In order to benchmark the four possible geometries generated by *VoxelMages*: quadric-based, voxelized, DICOM-RT, and DICOM-based, several benchmark cases have been carried out in order to find any unexpected discrepancies between them. To reduce the statistical uncertainty, at least 10^9 stories have been simulated in each test. We summarize some examples in the following subsections.

There are several approaches in the literature to compare 3D dose distributions and to make an estimation of possible systematic errors. In the following we will apply the formalism by Kawrakow and Fippel

(2000). Within this approach the possible discrepancies are quantified by evaluating

$$x_{ijk} = \frac{D_{ijk}^{geo_1} - D_{ijk}^{geo_2}}{\sqrt{(\sigma_{ijk}^{geo_1})^2 + (\sigma_{ijk}^{geo_2})^2}}, \tag{1}$$

where D_{ijk}^{geo} is the dose obtained using the geometry *geo* in a voxel with coordinates (x_i, y_j, z_k), σ_{ijk}^{geo} is the associated uncertainty, and $\sigma = \sqrt{(\sigma_{ijk}^{geo_1})^2 + (\sigma_{ijk}^{geo_2})^2}$ is the combined statistical uncertainty. The Kawrakow and Fippel approach assumes that x_{ijk} can be written as a sum of two sources of error, one associated with statistical uncertainties and another one comprising all sources of systematic uncertainties. Hence, by analyzing the distribution of x values one can determine whether it deviates from a Gaussian distribution, therefore implying the existence of systematic uncertainties. The simples realization of such approach, followed here, assumes that there are at most two uncorrelated sources of systematic uncertainties. Therefore it will provide the fractions α_1 and α_2 of voxels with systematic deviations Δ_1 and Δ_2, the remaining $1 - \alpha_1 - \alpha_2$ voxels showing no systematic deviations.

3.1. From quadric geometries into voxelized geometries. Benchmark

To benchmark the voxelizated geometries created by *VoxelMages* from the constructed quadric geometries two different scenarios have been designed. The first one will correspond to the geometry shown in Fig. 4(a) and named Benchmark I. This geometry is constructed only using boxes. Situated at the center of the lower box, there is a source of photons directed upwards. We have chosen this figure because a voxelized geometry (based on cubic voxels) should match exactly the quadric-based one. This simulation permits us to establish that the voxelized file are created according to the PENELOPE standards. The second benchmark simulation is a far more complex geometry designed to test whether *VoxelMages* is able to voxelize complex geometries where several interlinked bodies are present. This simulation, see Fig. 4(b), mimics the lower abdominal cavity, where the prostate gland, bladder, urethra, and lower part of the rectum are displayed. The interstitial water-equivalent material is not shown. This benchmark has been simulated in two different clinical situations. In the first one, Benchmark II.1, a brachytherapy seed mHDR-v2 (Elekta Brachytherapy, Veenendaal, The Netherlands) (Granero et al., 2011) was positioned inside the prostate. In the second one, Benchmark II.2, a typical clinical 6 MV photon beam spectrum is incident from the right. In this case the abundance of spherical surfaces makes that some systematic discrepancies are expected. A voxel size of 1 mm^3 has been used to voxelize both benchmark geometries..

Using the Kawrakow and Fippel formalism described above, it is found that the case Benchmark I shows no systematic deviations ($\alpha_1 = \alpha_2 = 0$) while for Benchmark II.1 a 32.8% of the voxels have a systematic deviation of 0.5σ, a 34.8% one of 0.8σ and 32.8% of the voxels have only statistical fluctuations. On the other hand, for Benchmark II.2 only a 32.7% of the voxels have a systematic deviation of 0.4σ, and the rest have only statistical fluctuations. As explained before, in both cases these small deviations appear only when cubic voxels try to reproduce curved surfaces. Therefore, it can be concluded that the geometry was correctly voxelized and both simulations are fully compatible.

3.2. DICOM image processing into voxelized geometries. Benchmark

In order to benchmark the DICOM importing feature, an artificial DICOM image has been produced using the geometry shown in Fig. 5 and then imported and voxelized using *VoxelMages*. In addition, this geometry has been also created using quadric surfaces and then voxelized as described in Section 3.1. This benchmarking scenario consists on three displaced spheres of different materials and radii

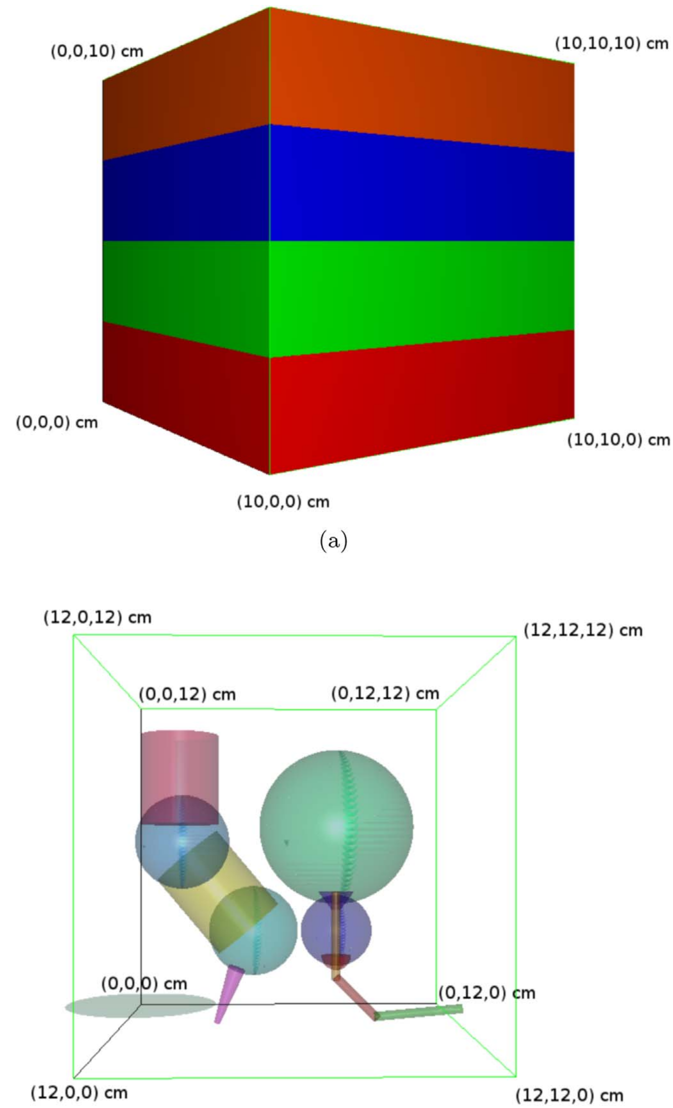

Fig. 4. Geometry of the Benchmark I (a) and II (b) simulations.

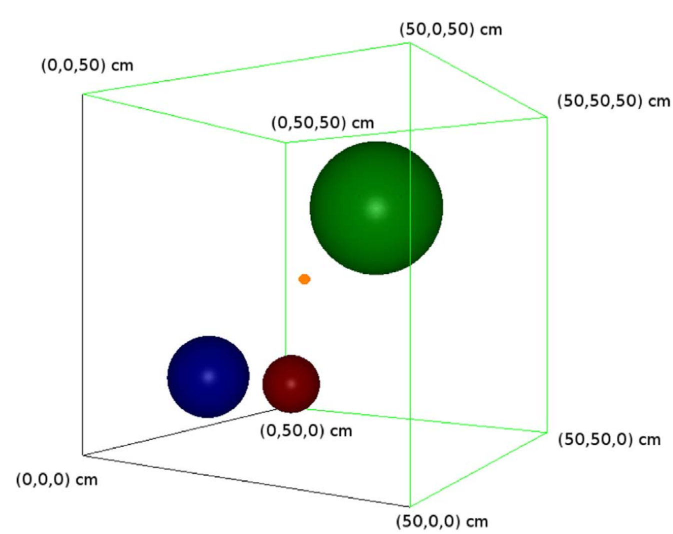

Fig. 5. The geometry used for testing the DICOM loader consisting of three spheres of different materials and radii. The orange point represents the isotropic photon source. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

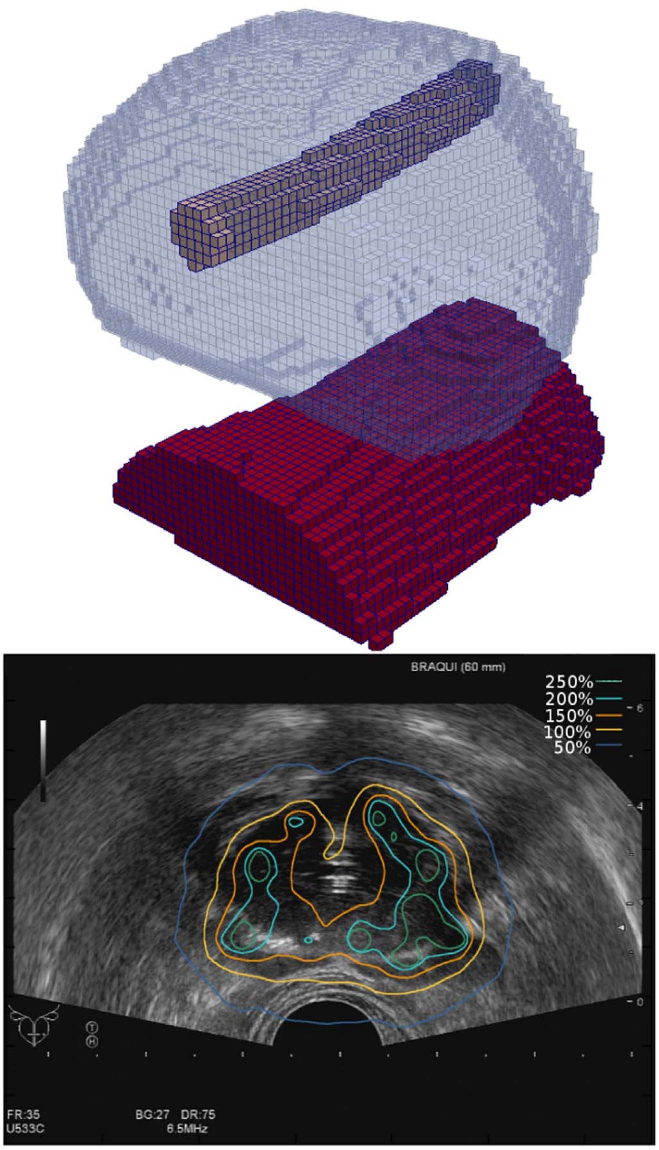

Fig. 6. (left) voxelized geometry generated by *VoxelMages* from the information given in the DICOM-RT and calibration file. Light blue voxels correspond to the prostate, brown voxels to the urethra and red ones to the rectum. (right) A US slice where isodoses have been superimposed. Dose has been normalized to the prescribed dose (160 Gy). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

inside a water phantom containing an isotropic photon source at its center..

By running the same simulation using both geometries and applying the Kawrakow and Fippel formalism one obtains that 21.3% of the voxels present a systematic deviation of 1.3σ. The reason for these small deviations can be traced back to volume averaging effects in the spheres surfaces due to the fact that the voxelization geometry and the one created importing the artificial DICOM image were chosen in this particular example with different voxel dimensions. Therefore, it can be concluded that both simulations are compatible and hence the program reads DICOM images and converts *HU* units correctly.

3.3. From DICOM-RT contours into voxelized geometries. Benchmark

To benchmark the capabilities of *VoxelMages* to import and create a simulation directly from a clinical plan, the University and Polytechnic Hospital La Fe has provided us with a low dose rate brachytherapy clinical plan in DICOM-RT format. In this plan 71 6711-OncoSeed™ seeds divided in 15 catheters were used in a prostate case. Therefore, the prostate will be the target of the clinical plan, while the rectum and the urethra will be the organs at risk.

The source geometry has been modeled using *VoxelMages* and consists of a 4.5 mm welded titanium capsule, 0.05 mm thick, with welded end caps. The capsule contains a 3.0 mm long silver rod onto which ^{125}I (mixture of AgBr and AgI in a 2.5:1 molecular ratio) is deposited. Details of the geometry can be found in Ref. Dolan et al. (2006). The strength of each source was 0.662 U for a total prescribed dose of 160 Gy applying the TG-43 formalism (Rivard et al., 2007). The planned D90 (maximum dose covering 90% of the volume) was 107%. The urethra has a D10 (maximum dose covering 10% of the volume) of 113% and the rectum a D2cc (minimum dose to the highest irradiated 2 cm^3 volume) of 68%. To explore *VoxelMages* material and volume identification algorithms, materials different from the mandatory full water volume inherent to the TG-43 formalism were chosen. Soft tissue (ICRP), liquid water, and soft tissue (ICRU) were chosen for the prostate, urethra and rectum respectively. The clinical parameters obtained were: 106% for the prostate D90, 124% for the urethra D10, and 68% for the rectum D2cc. Although they are within tolerance, the largest difference appear in the urethra D10 and can be traced back to two difference issues. The first one is the fact that a material different from water has been chosen for the prostate surrounding the urethra, hence differences in dose distributions are to be expected. The second one is that the automatic segmentation implemented in *VoxelMAges* assigns a voxels to a given volume when the voxel center is inside the contour. Hence the numbers of voxels assigned to the organs may differ from the ones chosen by the treatment planning system. This may be relevant in the case of small organs, like the urethra. The treatment planning systems has assigned a volume of 45.16, 1.59, and 13.46 cm^3 to the prostate, urethra, and rectum respectively. Those are to be compared with the ones assigned by *VoxelMages*, 45.79, 1.62, and 13.79 cm^3. We depict in Fig. 6 (figures not produced using *VoxelMages*) the voxelized geometry generated by *VoxelMages* from the information given in the DICOM-RT and calibration file (left) and a selected US slice where isodoses have been superimposed (right).

4. Conclusions

VoxelMages is a general-purpose graphical interface designed for creating complex geometries for general-purpose Monte Carlo simulations in an intuitive and simple way. Since the geometry can be visualized in a 3D viewer, errors made in the construction of the geometry can be easily detected and corrected. *VoxelMages* is able to import any DICOM image while at the same time transforming its *HU* units to mass density and assigning the corresponding materials. It also allows to import contouring data from a clinical plan in DICOM-RT format and, in the particular case of brachytherapy clinical plans, the location of the radioactive seeds. Moreover, *VoxelMages* allows the user to select the region to be simulated and export the selection in a format ready to run the simulation using the PENELOPE MC suite. It has been designed under an Open source license and therefore it does not require any proprietary software.

Acknowledgments

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