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2010 Phys. Med. Biol. 55 N211

(http://iopscience.iop.org/0031-9155/55/8/N03)

IOP PUBLISHING PHYSICS IN MEDICINE AND BIOLOGY

Phys. Med. Biol. **55** (2010) N211–N220 doi:10.1088/0031-9155/55/8/N03

NOTE

Linking computer-aided design (CAD) to Geant4-based Monte Carlo simulations for precise implementation of complex treatment head geometries

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Received 9 November 2009, in final form 10 February 2010
Published 26 March 2010
Online at stacks.iop.org/PMB/55/N211

Abstract
Most of the treatment head components of medical linear accelerators used in radiation therapy have complex geometrical shapes. They are typically designed using computer-aided design (CAD) applications. In Monte Carlo simulations of radiotherapy beam transport through the treatment head components, the relevant beam-generating and beam-modifying devices are inserted in the simulation toolkit using geometrical approximations of these components. Depending on their complexity, such approximations may introduce errors that can be propagated throughout the simulation. This drawback can be minimized by exporting a more precise geometry of the linac components from CAD and importing it into the Monte Carlo simulation environment. We present a technique that links three-dimensional CAD drawings of the treatment head components to Geant4 Monte Carlo simulations of dose deposition.

1. Introduction

Monte Carlo techniques for simulating radiation transport play a crucial role in medical physics (Andreo 1991, Rogers 2006, Chetty *et al* 2007) due to their ability to calculate accurate dose distributions for research in radiation therapy. One of the Monte Carlo packages that is becoming more popular in medical physics is Geant4 (Agostinelli *et al* 2003, Allison *et al* 2006, Carrier *et al* 2004), an object-oriented simulation toolkit with applications in different science areas, including nuclear physics, astrophysics, high energy physics, aerospace applications, etc. There are currently many Monte Carlo medical physics applications developed using

Geant4. Some of them are available freely to users as examples that accompany the installation of the toolkit[5]. Examples include the simulation of a medical linac, hadron therapy and brachytherapy, gamma therapy, DICOM file import interface, calculation of monoenergetic photon dose distribution in an ionization chamber and implementation of a human phantom. Other applications handle simulations of the accelerator's treatment head used for intensity-modulated radiation therapy (IMRT) (Foppiano *et al* 2004), the Leksell Gamma Knife (Romano *et al* 2007), the complex multileaf collimators (MLC) developed by Siemens (160MLC^{TM}) (Tacke *et al* 2006), proton therapy treatment planning (Aso *et al* 2004, Poon and Verhaegen 2005, Cirrone *et al* 2006, 2007) and PET/CT general purpose simulation platform (Strul *et al* 2003, Jan *et al* 2004). Time-dependent geometries can be simulated using Geant4 (Paganetti 2004), such as dynamic MLC motion, the rotational position of the range modulator wheel or the setting of the nozzle magnets.

Geant4 is particularly important for medical physics applications due to its flexibility in handling complex geometries (Tacke *et al* 2006, Paganetti 2004). Simulating the complex geometry of the linac's treatment head in great detail has a direct impact on the accuracy of dose distribution calculations (Tyagi *et al* 2007, Faddegon *et al* 2008). Several investigators have discussed the discrepancies between Monte Carlo build-up dose calculations and measurements for the 6 MV (Abdel-Rahman *et al* 2005) and 18 MV (Chibani and Ma 2007) photon beam medical linacs. These studies used Monte Carlo packages other than Geant4, i.e. EGSNRC and BEAM/DOSXYZ, respectively. In Chibani and Ma (2007), the discrepancies were found to be caused by inaccurate geometrical parameters of the primary collimator, the lead shielding collimator, as well as inaccurate geometrical representation of the IC-10 ionization chamber. By introducing a detailed geometry of an IC-10 ionization chamber in the simulation, it was shown in Chibani and Ma (2007) that the calculated and measured chamber responses were within 3% even at the zero depth. Geometry-related errors can be minimized through a computer-assisted procedure that transfers the geometry of the treatment head components from a CAD (computer-aided design) software to the Monte Carlo simulation environment. Exporting the treatment head design from the CAD software in a suitable file format, which can then be imported in the Monte Carlo simulation package, minimizes the errors which might be encountered during the manual assignment of the geometrical parameters of the treatment head components. In addition, material composition and density specification of the components have to be known in great detail, since variations in the density of the tungsten alloy used for the target block for example have been shown to modify significantly the 6 MV and 18 MV depth–dose curves (Keall *et al* 2003). The automated method presented here reduces the likelihood of the human error, both for geometrical parameter specification and material definition.

In this note, we present the methodology of linking electronic drawings produced with CAD software to the Geant4-based Monte Carlo package in order to preserve the geometrical complexity of the components needed in the simulation of the linac's treatment head for precise dose calculations. This detailed Monte Carlo model necessarily requires the researcher's access to sensitive proprietary information. Our procedure allows us to model not only the treatment head components in more complexity, but the components outside the field as well. We emphasize that our method is not restricted to medical physics since it can be applied to any other technical applications, such as aerospace engineering or high energy physics detector design, in which the precise implementation of the geometry and material specification are crucial to achieve the ultimate goal of high precision simulations. Other investigators

[5] The official page of the Geant4 organization is http://www.geant4.org/geant4/.

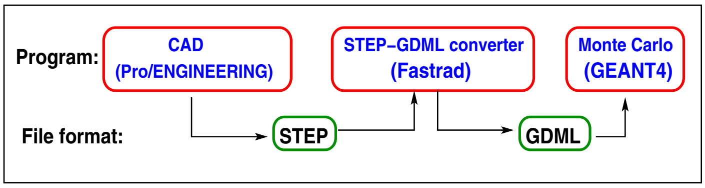

Figure 1. Flowchart of the methodology for linking electronic drawings produced with CAD software to the Monte Carlo simulation package to preserve the complexity of the geometrical shapes. The solid lines provide links between the type of program and the corresponding output file format.

have looked into achieving a CAD to Monte Carlo conversion, such as MCNPX-CGM, a coupling of traditional MCNPX with the Common Geometry Module (CGM) (Sawan *et al* 2007).

We also mention that, to our knowledge, this is the first example on how the exact treatment head geometry can be imported in a Monte Carlo simulation environment, opening the pathway toward accurate dose calculations using Monte Carlo methods.

2. Methods

The process for importing the exact treatment head geometry in the Geant4-based Monte Carlo package contains three steps. First, using a CAD software, the part drawing is exported as a STEP (STandard for the Exchange of Product) file. Second, the STEP file is converted in the Generalized Dynamic Markup Language (GDML) format which is compatible with Geant4. Third, the GDML file is imported in the Geant4 application. This strategy allows us to import into the Geant4 application any geometrical shape to a very fine approximation, set by the quality of the tessellation process during the STEP export. The methodology is schematically shown in figure 1. The flowchart shows the generic programs which are being linked, while the specific programs chosen in our case study are given in parentheses. The format of the output files for specific applications is indicated as well.

As a case study, we have selected several parts representing different linac treatment head components of relevance in Monte Carlo simulations, such as the vacuum window, target block, x-ray window, primary collimator, flattening filter, ionization chamber, shielding collimator, upper and lower jaws, the base plate and a half isocenter leaf. To execute the first step of the process outlined above, we have used Pro/ENGINEER Wildfire version 3.0 for Linux systems to generate the STEP files. STEP is an international standard for the computer-interpretable representation and exchange of product data (Fowler 1995, SCRA 2006). Its application protocol AP203 is used to exchange geometry, product structure and configuration management data. In what follows, we shall refer to the AP203 geometry representation as the STEP format. The STEP format provides a portable representation of the geometry within specified tolerances. The *solid* option was selected during the STEP export process in Pro/ENGINEERING. This is necessary in order to generate a tessellation which complies with the GDML specification. More precisely, the facets of the tessellation need to have their vertices oriented in a counterclockwise fashion as observed from the outside of the object, i.e. the unit vector of the facet points outward. This ensures that the interior of the object is well defined. OpenGL-based viewing drivers in Geant4 can easily spot an ill-defined tessellation by rendering it as a black surface.

Next, to export the STEP files in the GDML format, we have used Fastrad^{TM}(version 3.0) software[6]. GDML has been developed recently[7] (Chytracek *et al* 2006) for physics simulation and analysis purposes. It is essentially an application of XML (eXtensible Markup Language), a widely used application independent format. GDML is designed to describe geometrical data and the GDML files can be easily edited using any text editor. We mention that Geant4 is the only Monte Carlo code that currently has a GDML input module. Material assignments of individual parts were performed using the Fastrad^{TM}software as well. This step of the process is necessary since the information regarding the material composition is lost during the STEP export procedure. This issue is encountered not only in Pro/ENGINEERING, but also in other CAD software, such as SolidWorks or ST-developer. In principle, Pro/ENGINEERING could be queried to automatically provide the material specifications but is not currently available and therefore is susceptible to human transcription errors. In Fastrad^{TM}in particular, one can choose the material from the material list and modify it if needed. Using this procedure, a material XML file is created and associated with the exported GDML file. Alternatively, material specification can be performed in the GDML file, where the supported forms are simple materials (i.e. single elements) as well as mixtures composed on the basis of mass fraction or atom count.

Special attention must be given to complex assemblies which are composed of hundreds of individual parts. Many of these parts (i.e. pins, nuts, wafers, etc) are negligible in Monte Carlo simulations; hence, they can be eliminated from the CAD assembly. A good example of a complex assembly is the ionization chamber, whose relevant components in simulations are only the electrodes, the plastic windows and the outer body parts of the chamber. When we have exported all the components of the ionization chamber in a single STEP file, the output file was as big as 170 MB. However, after eliminating the unimportant components, we produced a simplified ionization chamber with only 2.3 MB. Therefore, a complex assembly can be reduced to a small number of parts which can then be handled easily in Fastrad^{TM}for material assignment, followed by the GDML export procedure. In the Geant4 simulation, the ion chamber is composed of simple parts, rather than assemblies, namely the patient side body, the target side body, three instances of the ion chamber window, two instances of the high voltage electrode, two signal electrodes and the support window. These are the important parts which intersect the beam path and contribute to radiation transport.

Once the GDML files representing particular treatment head components are generated, they can be imported in a straightforward manner (see footnote 7) in any Geant4 applications using the *G4GDMLParser* header file. We have worked with version 4.9.2 of Geant4, released in December 2008. For the visualization of the imported GDML files in Geant4, we have used the OpenInventor-based visualization driver. The import of the GDML files in Geant4 has been performed in the *DetectorConstruction* class, which is the typical class for the declaration and construction of the treatment head components. After the *G4GDMLParser* read in a particular GDML file and created an in-memory representation of its geometrical shape, we introduced a concrete instance of this shape and placed it into the reference frame of the overall treatment head. We repeated these steps for all the GDML files representing different parts of the linac's treatment head. In Geant4, any application performs the geometry loading only once, and then the transport of the particles is performed for a large number of runs to get good

[6] Fastrad radiation 3D CAD software is distributed by TRAD (France) http://www.trad.fr.
[7] GDML USERS'S GUIDE version 2.0 is available at http://lcgapp.cern.ch/project/simu/framework/GDML/.

statistics. Hence, following our procedure, little time is spent on detailed geometry loading compared to the time required for transporting the radiotherapy particles from the target block to the patient location or water phantom. It is important to emphasize that GDML not only allows complex and precise geometry implementation, but also the geometry can be modified without having to recompile the Geant4 application. This is also true for other Monte Carlo toolkits, such as MCNP[8] or MCBEND[9], which use text-based input for geometry, materials and sources.

Although the methodology described in this note has been applied successfully to the most important components of the linac's treatment head, we mention that we encountered some geometrical problems related to the tessellation of the flattening filter. We observed that while the STEP export file associated with the 6 MV flattening filter was correct based on a visual inspection performed in both Pro/ENGINEERING and other CAD viewers, once the file was tessellated in Fastrad™, two small depressions were generated in the tip region of the filter. While these geometrical problems in the tip region of the flattening filter could be observed by a careful visual inspection, we have measured the fluence map by placing a phase space immediately after the flattening filter and observed an enhanced particle accumulation effect in the central part of the map. Hence, for quality assurance purposes, fluence map calculations are recommended. This singular problem is most likely associated with Fastrad™. We did not observe similar geometrical problems with any other components used in this study. It is worth mentioning that we were not able to fix this problem because Fastrad™does not have the capability of generating the tessellation of a given geometry for a prescribed tolerance. It would be useful in the future to have access to a direct import of step files into Geant4 to avoid possible complications introduced by the tessellation process. In fact, a STEP interface was part of Geant4 version 5.2 and there is growing interest in reviving the STEP import module.

3. Results

We first show in figure 2 an example of how some of the treatment head components, the upper jaw and the half isocenter leaf of the multileaf collimator (MLC), are seen in Fastrad™ where the GDML export is performed (panel a) and in Geant4 where we import the GDML file and produce an output picture using the OpenInventor visualization driver (panels b–e). The geometrical specifications of the treatment head components are preserved during the transition from the CAD environment to the Monte Carlo environment. Note that even for this relatively simple objects, our procedure let us distinguish specific geometrical details, such as the canal for the shaft of the crossbar used to position the jaw and the mounting holes for the pins and screws (panel c), and also the variable thickness toward the bottom outer edge of the jaw (panel d). This geometrical complexity is not available in other Monte Carlo toolkits, such as BEAMnrc, where the jaws are represented by a set of paired bars[10].

To give a quantitative description of the time scale of our geometry import in the Geant4 application, we recorded the time spent to load and visualize individual GDML components.

[8] The official website of MCNP, A General Monte Carlo N-Particle Transport Code, is http://mcnp-green.lanl.gov/index.html.
[9] The official website of MCBEND, A Monte Carlo program for general radiation transport, is http://www.sercoassurance.com/answers/resource/areas/shield/mcbend.php.
[10] The official website of BEAMnrc: A Monte Carlo Simulation System for Modeling Radiotherapy sources, is http://www.irs.inms.nrc.ca/BEAM/beamhome.html.

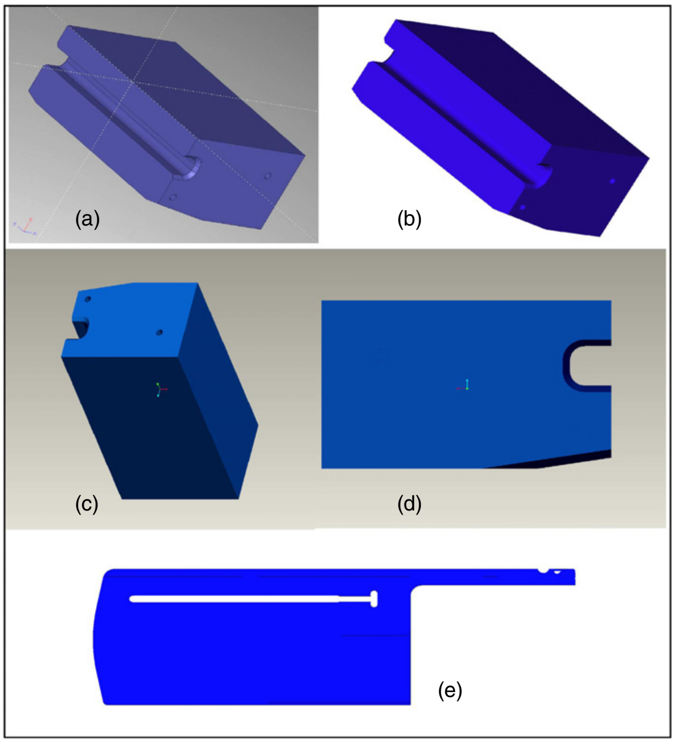

Figure 2. Visualization of the upper jaw in Fastrad^{TM}(a) and Geant4 using OpenInventor (b). Panel (c) shows the mounting holes. Panel (d) is a side view of the jaw which shows the canal of the crossbar and the variable thickness of the jaw. Panel (e) shows a half isocenter leaf.

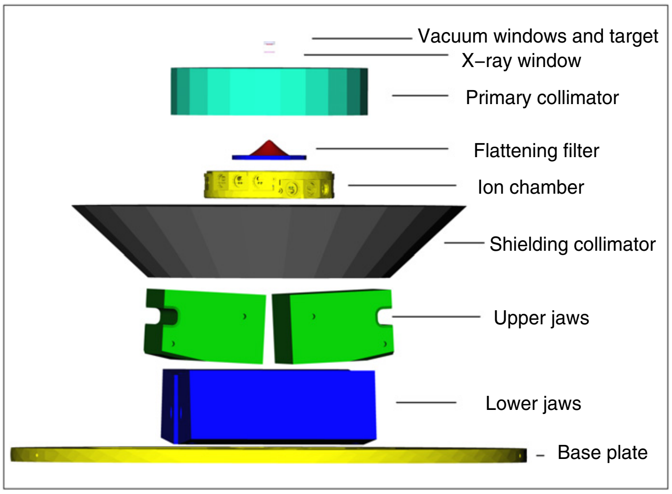

Figure 3. Visualization of the treatment head components using OpenInventor in Geant4. All the components have been imported in Geant4 as GDML input files.

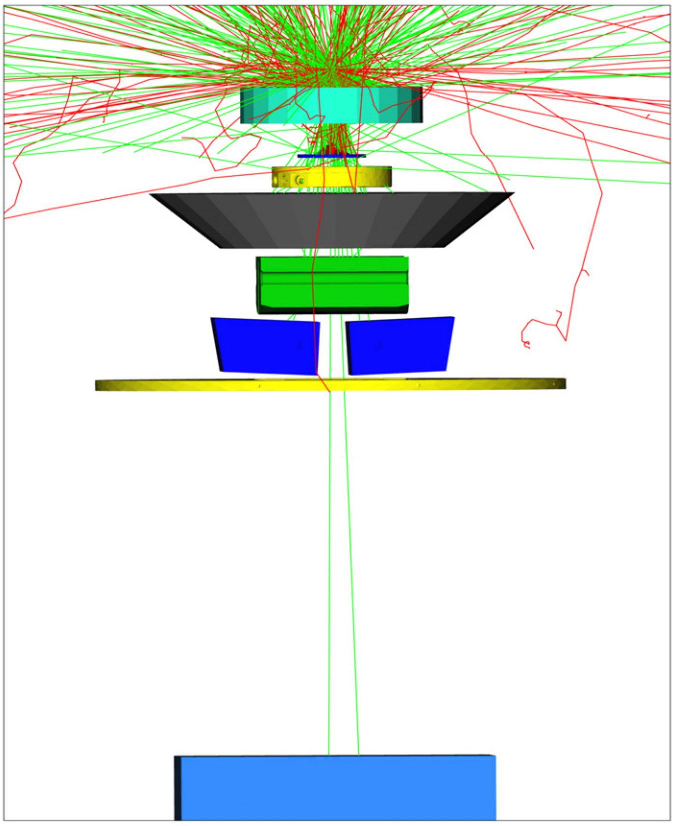

Figure 4. Visualization of Geant4 particle trajectories along the treatment head components using OpenInventor. Electrons and photons are shown in red and green, respectively. The field size was set to $10 \times 10\,\mathrm{cm}^2$ and the source-to-surface distance to 100 cm. Note that for proprietary reasons, the appearance of some of the components in this figure has been modified.

Their file sizes are indicated as well. The results are presented in table 1. The total time indicated here represents the time spent by our Geant4 application to read in the GDML file and create the geometrical object in the memory. We note that most of the simple GDML components can be loaded in approximately 10 s, while more complicated components with a large number of profiles and holes, such as the base plate, are loaded in about 50 s. We also note that the small GDML files (<200 KB) are loaded quickly, while the larger files (>2 MB) require more time to be loaded into Geant4. Overall, the entire treatment head is constructed in the Geant4 application and visualized with OpenInventor in about 63 s. This time interval is very short, compared to the time required to run a Monte Carlo simulation in which a large number of particles are transported through this complex geometry and recorded in the water phantom.

In figure 3, we present the result of loading the treatment head geometry in the Geant4 application using OpenInventor for visualization. The components seen in figure 3 are the GDML files listed in table 1, imported in the *DetectorConstruction* class of the Geant4 application we developed. The coordinates of the individual GDML objects with respect to the mother volume were specified in the same class.

Table 1. Quantitative illustration of the time spent in the Geant4 application to read in and visualize the GDML components and the corresponding GDML file size. The last row indicates the total time needed to upload the geometry of the entire treatment head components.

Component	Loading time (s)	GDML size (kB)
Vacuum window	16.7	28.8
Target button	11.8	41.4
X-ray window	10.8	28.8
Primary collimator	12.2	171.4
Flattening filter	10.8	189.9
Ionization chamber	24.0	2300
Shielding collimator	30.3	1500
Upper jaws	10.4	54.9
Lower jaws	10.9	89.1
Base plate	49.1	2000
Half isocenter leaf	6.5	181.3
All components	63.2	–

Next, in figure 4 we display a simulation of 400 events corresponding to 6 MeV incident electrons generated using the phase space information from Parmela (Young and Billen 1996). The electrons pass through the vacuum window and hit the tungsten target button. The particle trajectories through the linac treatment head system are displayed using OpenInventor. The electrons are shown in red, while the photons are shown in green. We note in figure 4 that, as expected, only a very small fraction (≈0.5%) of the generated photons reach the water phantom (shown in light blue) placed at 100 cm from the source point.

4. Conclusions

In this note, we have introduced a procedure for linking CAD drawings to Geant4-based Monte Carlo simulations in order to implement detailed geometrical representations of the treatment head components. We have shown that the steps involved in the process are robust and lead to easy and successful geometry construction. This project was motivated by the need for precise geometry implementation in medical physics applications, a prerequisite for accurate calculations. The presented procedure involves the generation of GDML files associated with the complex geometrical shapes of the treatment head components. Although Geant4 is the only Monte Carlo package that currently has the GDML input modality, taking into account that the GDML files are platform independent and language independent files, it would be useful to have this modality in other Monte Carlo packages, such as EGSnrc or MCNP, in medical physics as well as in other areas of physics, such as astronomy and engineering, allowing improved accuracy and facilitating easier comparisons from one Monte Carlo code to another.

The focus of this work was to describe the CAD to Monte Carlo link. Further work will investigate the tradeoff in terms of accuracy and efficiency of using the very detailed treatment head geometry. One might question the efficiency of the procedure presented here since complex geometries can lead to time-consuming simulations. To avoid this problem and obtain significant improvements in the efficiency of photon beam treatment head simulations[11] (Chetty *et al* 2007), one can split the Geant4 application in two parts: (1) first, a treatment head simulation with complex geometry can be used to generate a patient-independent phase space which can be placed between the shielding collimator and the upper jaws; (2) next, another application reads in the phase space file and transports the particles through the patient-specific collimation system. Then, dose distribution can be recorded in a voxelized water phantom. Since the second part of the Geant4 application has simple geometry, it is expected to be fast and efficient.

Acknowledgments

This work was supported in part by Varian Medical Systems. The authors would like to thank the Geant4 user support group, in particular Gabriele Cosmo of CERN, for answering questions regarding the import of GDML files in Geant4 and for making the Geant4 GDML input possible.

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