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Research Article

Monte Carlo Simulation of Cone X-ray Beam and Dose Scoring on Voxel Phantom with Open Source Software EGSnrcmp

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Abstract: Radiation is used nowadays for inspection, therapy, food safety, and diagnostic purposes. Our daily lives include the use of devices like airport scanners, projectional radiographers, CT scanners, treatment heads, cargo inspection systems, etc. However, these systems are extremely complicated and cost a significant amount of money to study, maintain and conduct research with. Monte Carlo is the ideal method for simulating such systems successfully and achieving findings that are remarkably comparable to experimental methods. Simulation software, however, is not always free, open source, and accessible to everyone. Open source software has gained popularity in the technological age that best represents the period we are living in, and practically all significant software sectors now use open source software tools. With the aid of an open-source, thoroughly validated software, called EGSnrcmp we were able to describe an abstract model-geometry of a cone-beam computed tomography X-rays source, produce patient-specific phantoms and score dosage values based on characteristics of the cone beam source. We outline the necessary methods and provide useful details about how to conduct such studies inside the software's ecosystem. Our study focuses on the relationship between the cone-beam source's field of view (FOV) and its impact on patient dosage, by emulating a CBCT examination. To characterize our cbct source, we employed stainless steel material to build the collimator and tungsten (W) material to build the anode. The most frequent energy at which these tests are conducted is 100 keV, which is the energy of the electrons we utilize. We were able to score absorbed dosage within a phantom produced from dicom images of a real patient, demonstrate the relationship between the FOV of the beam and the absorbed dosage and verify the cbct source using theoretical values.

Keywords: ***Medical Imaging; Monte Carlo; Open-source; Simulation; Software; Spectral distribution***

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1. Introduction

Several things have altered since radioactivity was discovered. We have managed to learn more about radioactivity and radiation in general. Each day we use radiation for all sort of applications in the field of medicine, food industry, security, energy and weapons production. In our study we are focused on X-rays for medical imaging, especially X-rays that form Beams that spread with Conical form used in Computed Tomography. Cone-Beam Computed Tomography CBCT can be used for various applications such as treatment planning [1], dental orthopaedics [2] etc.

Monte Carlo method is another way that solves deterministic problems by a stochastic approach utilizing random numbers as a baseline. In the plurality of applications and software working with the

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Monte Carlo method, the physical experiment can be accurately replicated. The geometry, the system's parameters and physics phenomena needs to be characterized using known statistics with extensively recorded values of their probability functions.

Several Monte Carlo software packages have been developed and allows us to do experiments in the domain of medical applications that utilizes radioactive materials, X-ray and gamma beams [3]. There is general purpose software such as MCNP [4], EGSnrcmp [5], Geant4 [6], Topas [7] and some application specific purpose such as Gate [8], Gamos [9], Serpent [10], etc. Some software is open-source and free and some require licensing, some are easy to use and some require good developing skills. For our research we chose the open-source general purpose EGSnrcmp software package. EGSnrcmp has more than 65 years [11] since it's development and can provide simulations of linear accelerators, X-ray tubes, dose calculation on voxelized geometries, dose calculations on RZ geometries etc.

The flexibility provided by EGSnrcmp is unique because it lets you describe your geometry, edit your physics parameters, score particles in three dimensional space, edit your results, create voxelized phantoms and much more. All these processes can be done inside the EGSnrcmp ecosystem without the need of external software packages for the data editing. Also the EGSnrcmp provides a friendly graphical user interface. After extensive research we came to the conclusion that the best software for our needs was EGSnrcmp due to its capabilities, autonomous layered design, and open distribution.

In modern external radio-therapy more and more linear accelerators (linacs) are modified by embed a CT system with a cone beam source (CBCT) in order to perform effective image-guided radiotherapy (IGRT) [12], so the patient needs to undergo one or multiple CBCT examinations before actually doing the radiotherapy with the linear accelerator. The patient thus actually is receiving more radiation exposure than calculated. Because before doing radiation therapy, doctors perform cbct scanning, in order to match the dicom image received before the treatment planning, with the image right before the treatment is being carried out. Of course, we need to point that the typical cbct in these particular exams is producing X-rays of around 30-150keV, whereas the typical linac is producing X-rays of 6-20MeV. So many attempts have been made with actual methods to determine just how much more extra exposure is the patient receiving from the cbct examination right before the radiation treatment. Most of these methods are using thermoluminescent (TLD) or mosfet dosimeters [13] but in recent years such calculations are performed via monte carlo especially in patient-specific dose calculations [14] and slowly opening the way to Monte Carlo simulation in clinical use.

Every day, many medical operations are carried out and a ton of data is generated. Software developers designed the Digital Imaging and Communications in Medicine (DICOM) standard to provide a standardized framework for storing, transferring, and encrypting image and patient data. We must understand that in medicine there are a lot of examinations and it is hard to create an abstract model for each purpose so it is nice to have some sort of standard and like DICOM [15]. In our work we use DICOM images of CT examinations which describes the body of an individual in a voxel array in three dimensions, containing Hounsfield units (HU) values.

The X-ray source, which creates the beam by converting fast electrons to braking radiation and is one of the factors that significantly affects the dose received from CT and CBCT examinations. EGSnrcmp is capable to perform simulations of modern X-ray tubes [16], perform half value layer calculations [17], dose scoring on patient-specific phantoms [18-19], etc.

Several studies have been conducted that imply that there is a direct relation of the X-ray beam's field of view (FOV), the voxel size and radiation dose [20-21]. These investigations were carried out using CBCT scanners, which irradiated a phantom with detectors on different modes of the scanner and displayed the dosage differences correspondingly. We were able to underline the association between Beam's FOV and absorbed dosage thanks to the work of Fatima M. Jadu [20] and Helena Aguiar Ribeiro Nascimento [21]. We are unable to directly compare our results with those of Fatima and Helena due to a lack of information regarding the CBCT scanners, X-ray tube assembly, scanner operational modes, phantom assembly, phantom geometry, tld detectors employed, and so on. Most of the time, manufacturers do not reveal such facts. The main concept is to run a Monte Carlo simulation to generate the various beams, varying only the FOV parameter, and then run another Monte Carlo simulation to calculate the dosage on individualized phantoms. Our approach is based on the ability of the software to effectively simulate X-ray Beams and effectively simulate dose calculations on personalized phantoms. In our work we are demonstrating the features of EGSnrcmp software to produce the appropriate cone beams with different FOVs, create voxelized phantom based on real human's organ geometries and score dosage. We display the software's capabilities, how to effectively use it while illustrating the connection between dose and FOV.

Although our technique is primarily based on computational calculations, it is unique in that it focuses solely on the link between Beam's FOV and Absorbed dosage, which is frequently overlooked or ignored. Our technique was not found anyplace else, either experimentally or computationally.

2. Materials and Methods

Due to the fact that our approach consists of multiple simulations we have introduced the term study. In order to complete a study, we divided it in to a series of simulations and processes of EGSnrcmp. To perform one complete study, we would need firstly to perform a BEAMnrc simulation to produce the cbct beam, with the desired field of view, secondly, we would use the ctcreate routine to produce the phantom and thirdly we would perform a DOSxyznrc simulation to calculate the absorbed dosage utilizing the results of the previous two processes. In figure 1 we present the work flow diagram of a complete study.

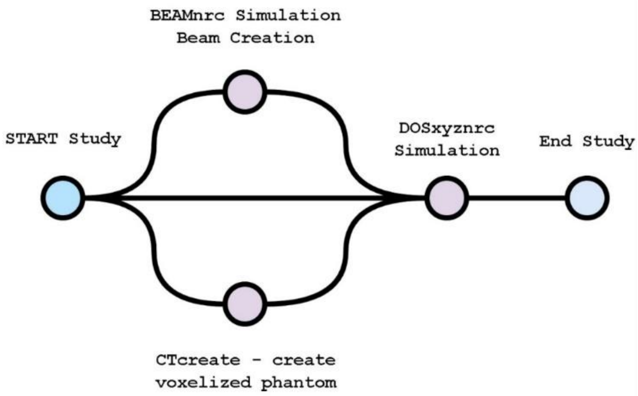


Figure 1. Work flow diagram of a complete study

2.1. BEAMnrc Simulation

In this simulation we utilize the routine of EGSnrcmp called BEAMnrc, so that the cone-beam source can be created. For the CBCT source we used the routine's geometrical components XTUBE, SLABS, CONS3R and SLABS to fully describe the 3D geometry this system.

The first component XTUBE is a geometrical component that describes the X-ray tube anode-target, it consists of tungsten (W) material as the target, its atomic number is Z=74, has an angle of 22^o [22]and this component is essential as it produces braking radiation (characteristic photons) that passes by all other components. At the last component the scoring of phase space file is being carried out. This component is bombarded by electrons from a 90^o angle from the side (x-direction). This is achieved by utilizing the "ISOURC 10 - "Parallel circular beam incident from the side", from the BEAMnrc process list. This component has dimensions in the xyz directions as follows, x=10mm, y=200mm, z=10mm. The target is inside vacuum, which covers it before and after the target.

The second component is SLABS and it describes a gap of vacuum and a gap of air. The dimensions of the vacuum gap are, x,y,z=400,400,20mm. The dimensions of the air gap are x,y,z=400,400,10mm respectively.

The third component is CONS3R and it describes our primary collimator, it consists of stacks of cones and needs 2 marks to define that particular geometry, so we chose R1=25mm and R2=55mm, the dimensions of this module are x,y,z=400,400,50mm. In the middle where the cone is defined the material used is vacuum and on the outsides of the cone the material is stainless steel.

Lastly the last component is SLABS and describes an air gap where at the bottom of it the particle scoring is being carried out. The last air gap dimensions are x=400mm, y=400mm and in the z dimension between 1mm-400mm, this is due to the fact that we need to investigate where the scoring is being done to produce the appropriate field of view (FOV) of the beam. Figure 2 describes the projection XZ of the 3D geometry of the BEAMnrc simulation.

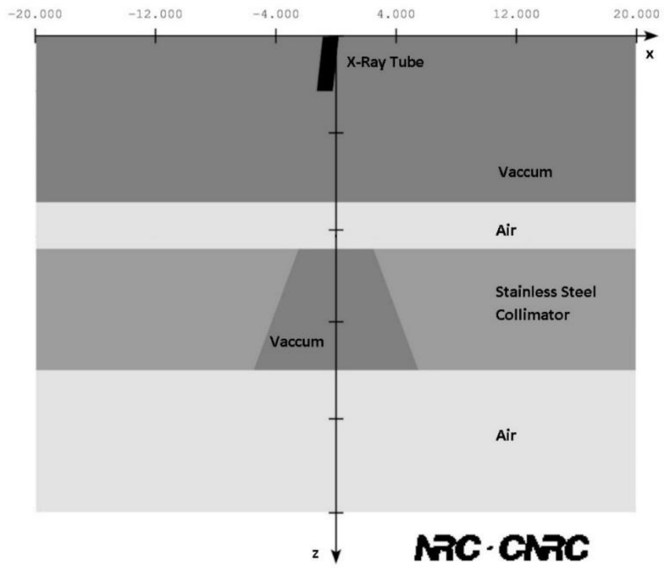


Figure 2. BEAMnrc 3D geometry setup, XZ projection

To begin the simulation process, we need to set our parameters of the 3D "World", the physics processes, set up the cut-off energies and the energy transfer threshold for the particles involved. The world's material was set to "AIR", while the thresholds and cut-off energies for electrons were AE=0.511MeV and ECUT=0.660MeV and for the photons was set to AP=0.001MeV and PCUT=0.105MeV. To make our simulation faster we have utilized an optimization method called variance reduction. EGSnrcmp ecosystem provides a function called DBS (directional bremsstrahlung splitting) which enriches the probability of the bremsstrahlung phenomena in any direction. The result was that our simulations run faster by up to 30 times [23]. Because the program is using random number generators (RNG) we need to provide two random seeds, seed1=33 and seed2=97. At table 1 we can see all the physics parameters that were utilized to make these simulations taking in to account all physics and optimizations of the software's routine.

Table 1. BEAMnrc Parameters list

MC-Parameter	Values
Bremsstrahlung Splitting	Directional
Maximum step size (cm)	10
ESTEPE	0.25
Xlmax	0.5
Boundary crossing algorithm	EXACT
Electron-step Algorithm	PRESTA-II
Spin effects	On
Bremsstrahlung angular sampling	Koch-Motz
Bremsstrahlung cross sections	NRC
Bound Compton scattering	On
Pair angular sampling	Koch-Motz
Pair cross-sections	NRC
Photoelectron angular sampling	On
Rayleigh scattering	On
Atomic relaxations	On
Photon cross-sections	Xcom
Incident particle	Electron
Source number	ISOURC10
Beam radius	0.2mm
Source beam energy-Monoenergetic	Kinetic energy = 0.100 MeV

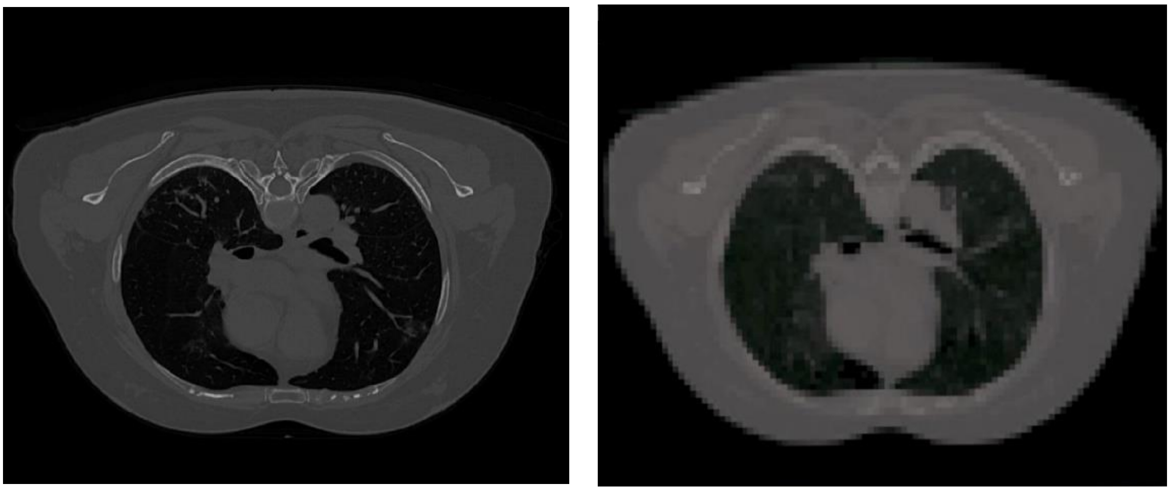
2.2. EGS-Phantom Creation.

In this process we utilize the ctcreate [24] routine in order to read all dicom slices (dcm) of the exam image file and produce the egs-phantom, so that later on we are able to score dosage. From an open source dataset of anonymous patient chest examination images [25] we obtained an image with voxel array size of x=512, y=512, z=250 of total 65,536,000 values, with each voxel having x=1mm, y=1mm, z=1mm voxel resolution. The routine lets us associate each original array value of hounsfield units (HU) to a value of material, that we need to define, and a value of density (g/cc). We used four materials air, lung, tissue and bone. Each of these materials is a compound of different elements, in table 2 we show the consistency of elements associated for each material.

Table 2. Material consistency of elements

Material	Element	Atomic number (Z)	Percentage
Air	Carbon (C)	6	0.02%
	Nitrogen (N)	7	75.52%
	Oxygen (O)	8	23.18%
	Argon (Ar)	18	1.28%
Bone	Hydrogen (H)	1	4.72%
	Carbon (C)	6	14.43%
	Nitrogen (N)	7	4.20%
	Oxygen (O)	8	44.61%
	Magnesium (MG)	12	0.22%
	Phosphorus (P)	15	10.50%
	Sulfur (S)	16	0.31%
	Calcium (CA)	20	21.00%
	Zinc (ZN)	30	0.01%
Lung	Hydrogen (H)	1	10.30%
	Carbon (C)	6	10.50%
	Nitrogen (N)	7	3.10%
	Oxygen (O)	8	74.90%
	Sodium (NA)	11	0.20%
	Phosphorus (P)	15	0.20%
	Sulfur (S)	16	0.30%
	Chlorine (CL)	17	0.30%
	Potassium (K)	19	0.20%
Tissue	Hydrogen (H)	1	10.12%
	Carbon (C)	6	11.10%
	Nitrogen (N)	7	2.60%
	Oxygen (O)	8	76.18%

Utilizing the CT ramp function, with default parameters we were able to create the egsphantom, however the software can't have such good voxel resolution array size. So, the egs-phantom has voxel array size of x=125, y=125, z=125 with total of 1,953,125 values and the voxel resolution the program allowed is x=4mm, y=4mm, z=2mm. Thus, the resolution of the phantom has been reduced compared with the original file. Figure 3 depicts the examination DICOM file and the egs-phantom file produced.



a b

Figure 3. a) Examination DICOM (dcm) file slice, b) egs-phantom file slice

2.3. DOSxyz Simulation.

After generating the egs-phantom and the cone beam we want to configure DOSxyz software routine in order to score dosage in the phantom utilizing the beams produced. Our intension is to simulate a CBCT examination so we take the output files from the previously BEAMnrc simulations, by selecting "ISOURC-8=Phase-space source from multiple direction ", option inside the DOSxyz option list. We managed to have multiple projections of the cone beam. Figure 4 depicts how the source is irradiating.

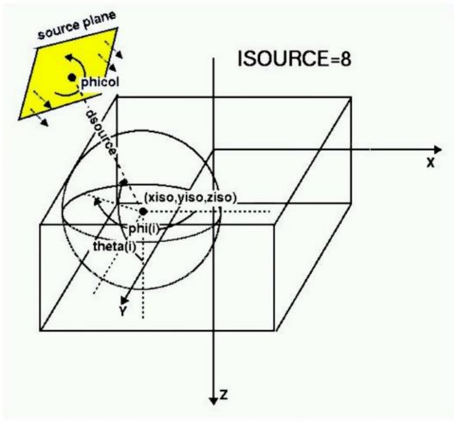


Figure 4. DOSxyz ISOURC=8 option's paremeters [24]

To accomplish that we defined the isocenter with coordinates x,y,z=250,250,130mm, the distance from the isocenter dsource=250mm, angle theta had a fixed value of theta=90^{o} and we vary the phi angle from 0^{o}-356.6^{o} in order to accomplish a 360^{o} rotation and have 100 projections with equal probability and angle of 3.6^{o} each. The values of the random number generators seed were seed1=30 and seed2=85. Table 3 describes all parameters that were used in order to perform the simulation with the highest standards.

Table 3. DOSxyz Parameters list

MC-Parameter	Values
Maximum step size (cm)	10
ESTEPE	0.25
Maximum first elastic scattering moment per step	0.5
Boundary crossing algorithm	EXACT
Electron-step Algorithm	PRESTA-II
Spin effects	On
Bremsstrahlung angular sampling	Simple
Bremsstrahlung cross sections	Bethe-Heitler
Compton cross sections	Default
Pair angular sampling	Simple
Pair cross-sections	Bethe-Heitler
Photon cross-sections	Xcom
Incident particle	Photon
Source number	ISOURC8
Number of Projections	100
Angle of rotation of each projection	3.6^{o}
Photon splitting number	10

To be reassured that the source is irradiating the egs-phantom from all direction performing a 360^{o} rotation we plot a dosimetric map via the dosxyz_show routine [26] and saw that it met our expectations. Figure 5 depicts the dosimetric map of inside the phantom, visualizing the dose distribution into regions, after the irradiation with the cone beam source. As it can be observed the phantom is irradiated from all directions parallel to the z-direction, just like in a CBCT examination.

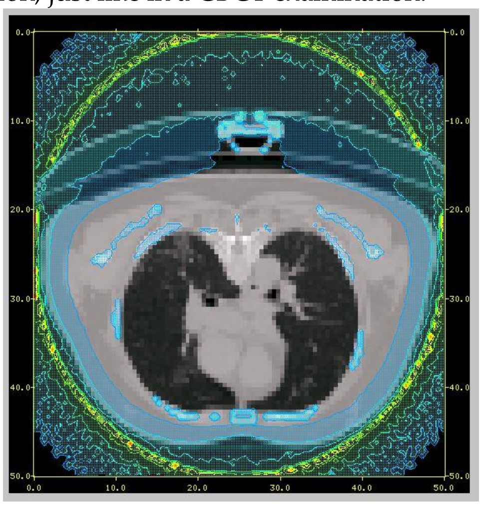


Figure 5. Dosimetric map slice

3. Results and Discussion

After defining a complete study, which consists of BEAMnrc simulation, phantom creation and DOSXYZnrc simulation, we present three cases of different cone beam's field of view (FOV), their photons distribution on the x-y plane and dosage results affecting four different regions of a patient's chest, namely heart, lungs, skin and spine. For the beams produced the initial particles used was $250*10^{6}$, that number was chosen after multiple runs and it was ideal number of initial particles due to the fact that it produced very small uncertainties in the results. The phase space files scored $60*10^{6}$ photons on each case having the size of approximately 2 gigabytes on the hard drive for each beam. All BEAMnrc's output files were analysed by BEAMDP [27] routine and plot graphs. For the DOSXYZnrc simulation the initial photon particles used was 10^{9} particles which was achieved by redistributing the phase space file. The DOSXYZnrc simulation produced dose output files which was further consumed by the STADOSE [28] routine to extract data information and help us further analyse the dose distributions, providing the option to graph plots. All plots from the beams simulations and the dose simulations, were produced by xmgrace [29].

For the whole study simulations, we utilize a modern computational unit with intel i7 10^{th} generation CPU, 16 gigabytes of random access memory (RAM) and 100 gigabyte of hard drive. Each complete study took about 20-24 cpu-hours to complete.

We did not use extra filtration on the anode target in order to test the abilities of the software to handle low energy photons spectra. From our investigation and continuous runs, we decided to choose three different FOVs, one of 70*100mm, second of 200*200mm and third of 360*360 mm. In Figure 6 we can observe the characteristic X-rays for the tungsten (W) material of the anode for each case of FOV. We can clearly see the L and K bands X-ray characteristics of the tungsten (W) target [30]. More analytically for the K band, a1, a2, b1, b2=0.057, 0.059, 0.067, 0.069 MeV and for the L band, a,b,c=0.012MeV. While the characteristic X-rays are in the same position the energy Fluence value is becoming lesser as the beam broadens, so the beam becomes less intense in terms of fluence per cm^2.

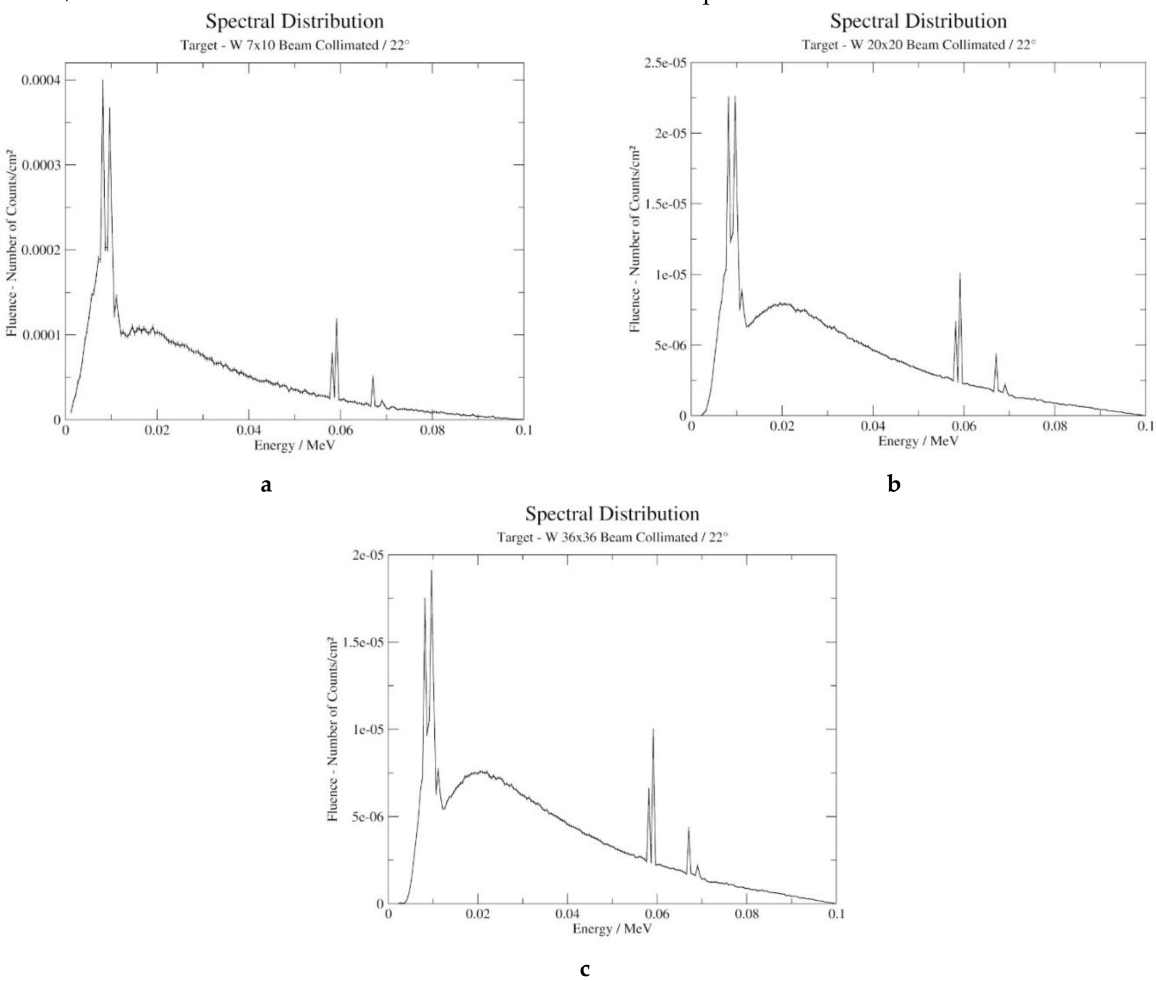


Figure 6. Spectral Distributions for each FOV case. a) 70*100mm, b) 200*200mm, c) 360*360mm

We derived the scatter plots for all cases to evaluate the beam as it passes via the collimator. In figure 7 we present the scatter plots for all FOVs. The number of particles we are plotting is 10,000 in order to have a clean scatter plot and observe the quality of the beams. Each particle is represented by a green snowflake symbol. Due to the heel effect we can clearly see slightly more particles being scored on the positive side of the x-axis than to the negative side.

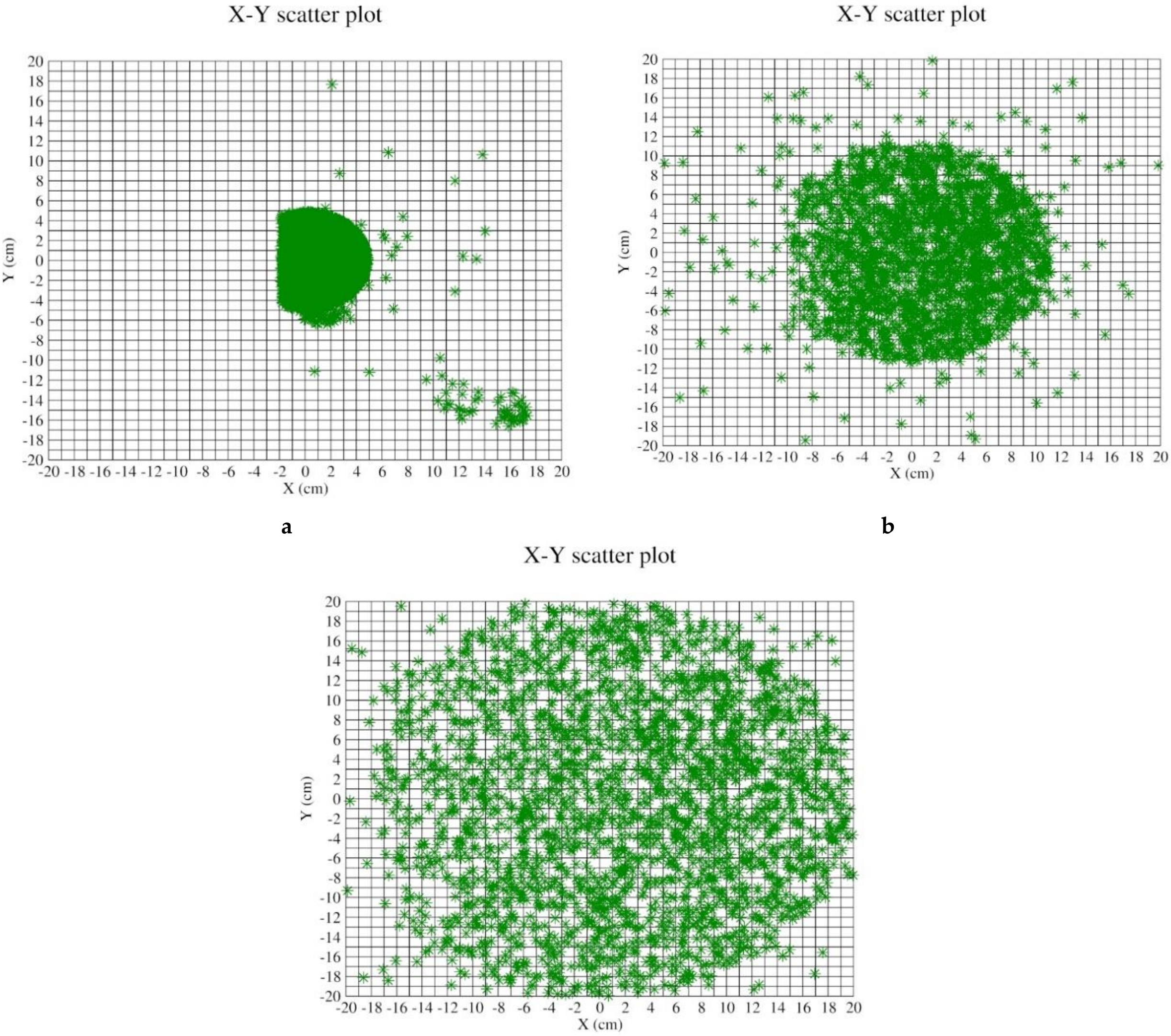


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Figure 7. Scatter plots for each FOV cases. a) 70*100mm, b) 200*200mm, c) 360*360mm

Lastly, we present the absorbed dose profiles of specific regions on the egs-phantom. We choose to evaluate the heart, lungs, skin and spine exposures. In Figure 8 we present the depth dose comparison profiles of the organ regions for the heart, the lungs, the skin and the spine bone.

As it can be observed the FOV of the beam serves a significant role on the absorbed dose scored. Taking into consideration that each simulation of the beam has the exact same parameters, the voxel size of the phantom is the same, the only difference is the field of view, we observe that as the beam spreads less dose is scored and thus less radiation is received by the patient. This factor is very significant because a lot of times when building scanning systems that utilize X-rays, not only the source of the scanner plays an important part to the end dosage received by the patient, but also the scanner's detectors and geometry of the system needs to be taken in to account, when building such scanners. In Table 4 we present the mean value of absorbed dose per photon in grey (Gy) values for each of the organ region.

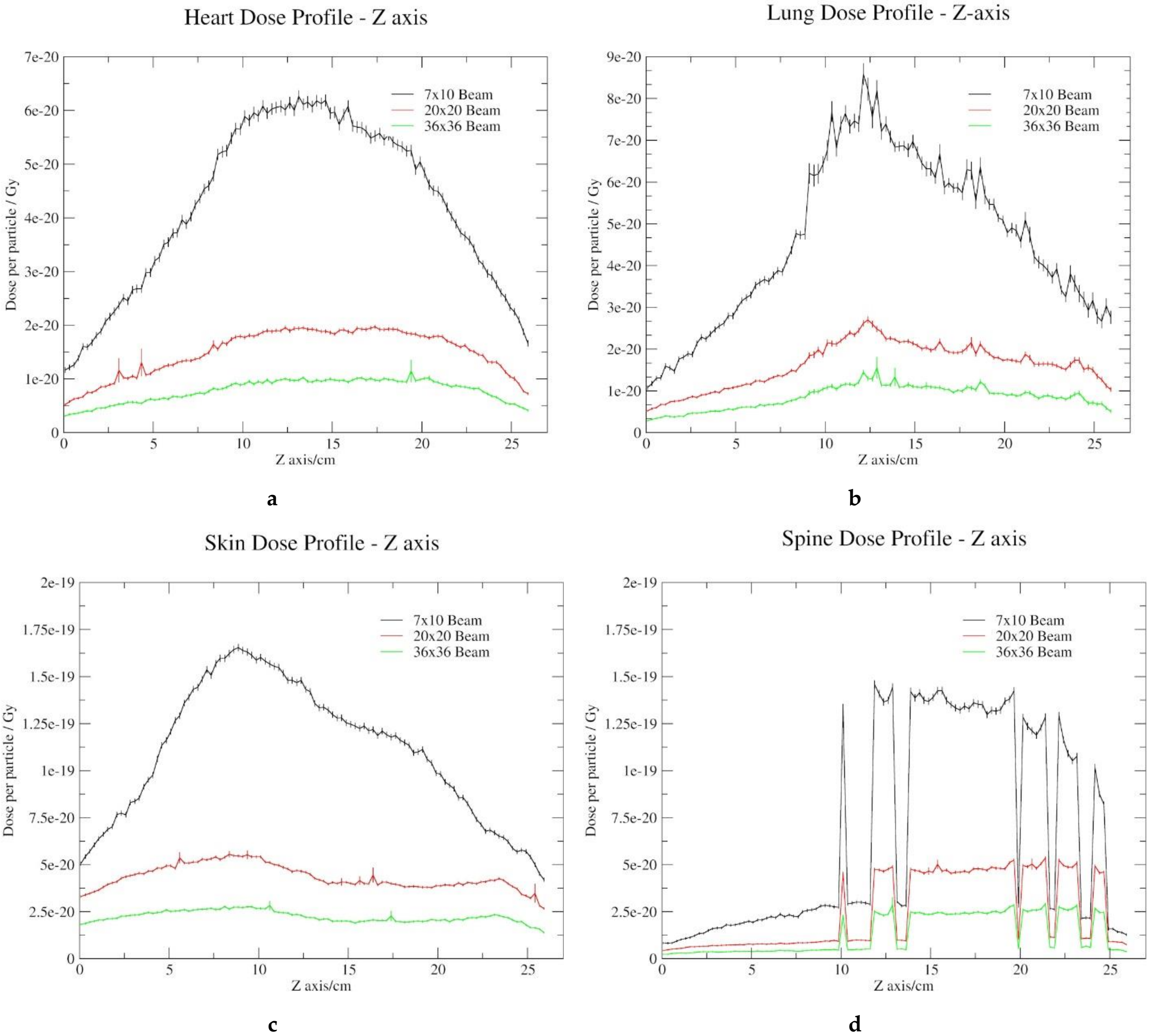

Figure 8. Dose comparison profiles with various FOVs. a) Heart, b) Lung, c) Skin and d) Spine.

Table 4. Mean Dosage values per organ profile.

Organ	Beam's FOV	Mean Dose per photon/Gy
Heart	70x100 mm	$4.23*10^{-20} \pm 8.60*10^{-22}$
	200x200 mm	$1.51*10^{-20} \pm 3.09*10^{-22}$
	360x360 mm	$7.82*10^{-21} \pm 2.02*10^{-22}$
Lung	70x100 mm	$4.64*10^{-20} \pm 1.34*10^{-21}$
	200x200 mm	$1.63*10^{-20} \pm 4.12*10^{-22}$
	360x360 mm	$8.48*10^{-21} \pm 3.26*10^{-22}$
Skin	70x100 mm	$1.10*10^{-19} \pm 1.43*10^{-21}$
	200x200 mm	$4.34*10^{-20} \pm 6.35*10^{-22}$
	360x360 mm	$2.23*10^{-20} \pm 3.77*10^{-22}$
Spine	70x100 mm	$6.67*10^{-20} \pm 1.09*10^{-21}$
	200x200 mm	$2.53*10^{-20} \pm 4.18*10^{-22}$
	360x360 mm	$1.31*10^{-20} \pm 2.88*10^{-22}$

4. Conclusion

Radiation is a part of our everyday lives and in the near future more and more breakthroughs will come. Already we are in an era where we can manipulate protons and neutrons in order to make new materials and medically treat people. Monte carlo software is already playing a significant role on medical and scanning equipment and little by little it will come to the treatment planning field in clinical use, so that people can be treated much more efficiently and be protected by extra radiation. Open source software for such experimentations is very crucial not only for developing, validating and optimize existing structures and models but also as a tool for education. Open source provides the infrastructure to teach people how such complicated systems work but also how people can contribute and help each other. We personally believe that open source software is the key to knowledge and in few years all software would become open as it is the trend of the last 15 years. Nonetheless in this work we were able to effectively utilize EGSnrcmp and the routines BEAMnrc and DOSXYZnrc in order to create a complete study, that goes from X-ray beam generation to dosage calculation, based on personalized phantoms. We validated our model of the CBCT beam and show the relationship between the beam's FOV and dose, on personalized data. With our study we evaluated EGSnrcmp ecosystem and showed that all the tools provided by the community are enough to conduct extensive and challenging investigations. Of course, because we are only exhibiting computer calculations, there are constraints, such as of the program EGSnrcmp that is confined to interactions between photons, electrons, and positrons. Beam quality and x-ray source optimization are other limitations in order for our model to match a certain CT scanner. There are limitations to personalized phantom creation, and higher quality results would be produced if more advanced models and computational phantoms that replicate an actual human body in more detail, both computationally and medically, were available. Unfortunately, most information about modern medical equipment is not provided by the industry's manufacturers and research is not only needed to simulate those systems but also to find the correct parameters, geometrical dimensions and components of those mechanisms. Lastly we were able to demonstrate a fairly substantial outcome, despite the fact that our models were abstract and basic since the link between the patient's dose and the FOV of an X-ray beam was not always evident, frequently ignored or not even acknowledged.

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Conflicts of Interest

The authors of the paper have stated no conflicts of any particular interest.

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