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PET image reconstruction and dosimetry from voxelized phantoms with GATE

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ABSTRACT

Accurate patient-specific internal dosimetry is a critical concern in the field of nuclear medicine. GATE is a robust Monte Carlo toolkit renowned for its integration of Geant4 algorithms, PET specialized tools and patient-specific dosimetry estimation. In this work, a GATE model is developed to simulate the PET scanner Biograph Vision and a voxelized phantom from Computed Tomography (CT) images. The segmentation of the CT images is performed using a deep learning model capable of automatically delineating anatomical structures, setting the basis for creating the patient-specific voxel phantom. GATE Nested parameterization method is employed for its efficient memory usage in defining geometry and faster navigation for ultra-large number of voxels. Simultaneously, PET acquisition data is used to assign the corresponding activity of a source to each voxel. This study aims to highlight the potential of GATE as a simulation tool within a methodology that integrates PET image reconstruction and internal dosimetry calculation, focused specifically on its application in prostate diagnostic testing via 18F-FDG. S-Value and dose are calculated for the prostate gland, yielding values of 1.52 E−4 mGy/MBq·s and 8.1 mGy, respectively, consistent with literature findings. Differences in S-Values with the ICRP Phantom and with OpenDose for surrounding organs range from 0.5% to 67.9%, which can be attributed to the choice of phantoms used in calculations. This work confirms the capability of GATE to reproduce clinical studies using anthropomorphic voxelized models.

1. Introduction

Computed Tomography (CT) joint with Positron Emission Tomography (PET) are widely used in current medical diagnostics. The integration of both techniques allows the simultaneous acquisition of anatomical and functional information in a single procedure. However, through direct measurements it is not possible to determine the radiation dose absorbed by the organs in these studies. Traditionally, internal dose assessments used pre-calculated reference data from anatomical models.

Dose calculations can be performed either at the whole-organ level or at the voxel level. At the whole-organ level, the Medical Internal Radiation Dose (MIRD) model simplifies patient anatomy using basic shapes like spheres or cubes, assuming uniform activity distribution within each organ. Conversely, personalized voxel-based dosimetry relies on CT imaging to generate 3D computational phantoms composed of small volume elements (voxels) providing information on tissue compositions, densities and attenuation maps. Concurrently, PET scans offer crucial data on activity distribution. However, it is important to note that the process of segmenting CT images and obtaining the phantom can be laborious and costly. While efforts have been made to automate this process, including the application of deep learning models, challenges remain in achieving accurate and efficient segmentation (Fu et al., 2021). In this context, due to the improvement in computing capacity and speed, Monte Carlo methods have gained relevance for dose calculation. Among others, tools like the GATE toolkit are widely used due to their capability to integrate anatomical data of the patient obtained from CT DICOM and the distribution pattern of the radiotracer from PET DICOM images facilitating the creation of voxelized geometries and sources.

S-values, expressed in $GyBq^{-1}s^{-1}$, refer to the mean absorbed dose to a given target per nuclear disintegration in a source region, establishing a relationship between a certain organ that contains a radionuclide and the surrounding tissues (Snyder et al., 1975). However, current

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literature shows significant differences between S-values in these personalized phantoms and standard ICRP models for similar case studies. Bakkali et al. (2022) present S-values in the prostate gland calculated with Monte Carlo InterDosi simulations in a Zubal voxelized phantom and the voxelized ICRP adult male phantom with IDAC-DOSE 2.1 code, ranging the relative differences from 10.74% to 86.62% depending on the radionuclide used. Reynoso-Mejía et al. (2020) compare the S-values of the ICRP-HEAD phantom with MCNP6 code to those in the MIRD-15 phantom and in the voxelized VIP-Man phantom, and obtain the ratios for eight source structures and eight target structures. In this work, ratios for ICRP-HEAD phantom/MIRD-15 phantom ranged from 0.21 to 10.39, and the ratios for ICRP-HEAD phantom/-VIP-Man phantom ranged from 0.48 to 1.48, depending on the tissue. These discrepancies highlight the limitations of standardized phantom-based data and underscore the need for personalized internal dosimetry using realistic patient anatomy for a more precise evaluation of potential risks while considering crucial radiation protection factors.

GATE is an application based on the GEANT4 toolkit (Agostinelli et al., 2003; Allison et al., 2016). GEANT4 handles the simulation of particle-matter interactions, while GATE offers extra features to simplify the creation of simulations using GEANT4. Developed by the OpenGate collaboration, GATE is community-driven, allowing users to access the source code and suggest new features. GATE has broad applications, especially in PET and SPECT studies, where it has been used to verify and validate commercial PET scanners (Jan et al., 2004; Kowalski et al., 2018; Peña-Acosta et al., 2024). The simulation models also offer the flexibility to adjust design parameters including the geometry, materials and digitizer, as well as to develop new conceptual scanners (Karakatsanis et al., 2022; Yamaya et al., 2011). Additionally, GATE has been extensively tested and utilized for dosimetry calculations. In the literature, several works review this potential of GATE (Papadimitroulas, 2017; Sarrut et al., 2014; Villoing et al., 2017; Visvikis et al., 2006), and specifically with voxelized phantoms (Gupta et al., 2019; Kaddouch and El Khayati, 2017; Kinase et al., 2011). In this context, leveraging anatomical data and the activity distribution within a patient, along with the GATE toolkit, may allow for optimization and interpretation of PET/CT images.

This study aims to highlight the potential of GATE as a simulation tool within a methodology that integrates a PET scan simulation, image reconstruction and internal dosimetry calculation.

2. Materials and methods

Tailored for nuclear medicine and emission tomography applications, the GATE toolkit has emerged as a versatile platform for system modeling and radiation transport simulation, garnering increasing attention in recent research. The calculations presented in this work involve obtaining reconstructed images from the anatomical information of the patient and the dose distribution resulting from the administration of 18F-FDG. The GATE model integrates the characterization of a Biograph Vision PET scanner to obtain coincidence data that is later reconstructed with CASTOR software (Merlin et al., 2018). Furthermore, leveraging the dosimetry calculation capabilities of GATE, absorbed doses are determined for the prostate gland and surrounding organs at risk, such as the urinary bladder wall, the rectum wall, and the pelvic bones.

2.1. Voxelized GATE model

A voxelized phantom refers to a three-dimensional representation of an object or organism divided into small volumetric elements. This representation enables accurate modeling of complex structures within a computational environment. Specific properties, such as density and material composition, are assigned to each voxel to simulate how radiotracers interact with the organism. This approach facilitates accurate and detailed simulations, allowing the calculation of dose distributions and other critical parameters for medical applications.

The PET/CT data used in this study were obtained from The Cancer Genome Atlas Prostate Adenocarcinoma (TCGA-PRAD) collection (Zuley et al., 2016), with its radiological data archived on The Cancer Imaging Archive (TCIA) (Clark et al., 2013). Data correspond to a 54-year-old male patient weighing 104 kg. For the development of a patient-specific phantom, CT images were segmented using a deep learning computational model called TotalSegmentator (Wasserthal et al., 2023), capable of automatically segmenting 107 anatomical structures from CT images. TotalSegmentator was provided to the authors as a pre-trained Python package, utilized in this study through a user interface available as an extension in the free and open-source software 3DSlicer (Fedorov et al., 2012). Selecting the “Advanced" option in the 3DSlicer extension allowed access to both trained models of TotalSegmentator. The “Fast" model was trained with CT images with a slice thickness of 3.0 mm, while the default model used images with a slice thickness of 1.5 mm, resulting in higher accuracy. The default model achieved a Dice similarity coefficient of 0.943 (95% CI [0.938, 0.947]) in the comparison of the predicted segmentations and the reference segmentations, which were approved by specialists in the training dataset of 1082 patients (Wasserthal et al., 2023).

The main approach to define material properties in GATE is via a material database. This database contains essential data that GATE utilizes to assign the corresponding properties from Geant4 datasets, and it can be readily customized by the user. Converting image data into material definitions in GATE entails assigning suitable material properties to each voxel-encoded value. This process depends on predefined material properties stored in the GateMaterials.db file. As segmented phantom data use ‘label values’, a range translator is used to convert these values into materials, with each voxel being assigned to a specific material if its value falls within the designated material range. Fig. 1 shows a 3D visualization of the segmented phantom for this study, in which 20 tissues and air have been used as materials (Fig. 1).

To simulate a PET scan with GATE, defining the irradiated geometry and specifying the source are essential steps, with the source modeling varying according to the application. In this study, a voxelized-type model was used, utilizing metabolic data of a patient as the source. A linear translation operation is conducted using GATE, which involves converting the intensities in the metabolic images into corresponding probabilities for a decay event to occur within a specific voxel, effectively translating image brightness into quantitative activity (Bq) based on simulated histories. Furthermore, the source was configured as ‘BackToBack’ type, emitting pairs of photons at 180° relative to each other. This setup is particularly useful in PET scan simulation in which 18F is used as a radioisotope since it simplifies the physic process by assuming that no radioactive decay and positron annihilation occur, reproducing only the emission of pairs of photons (511.0 keV for each

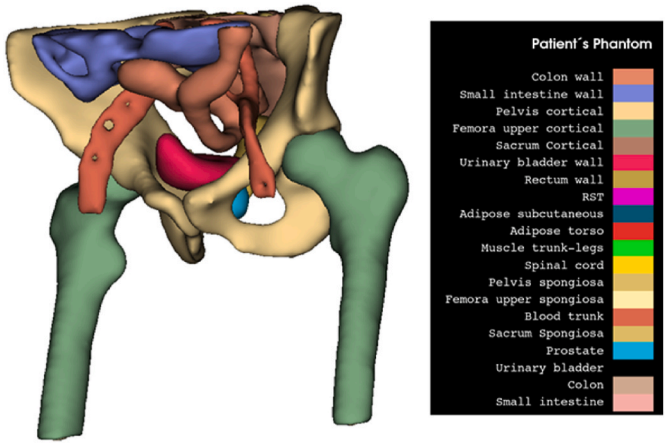

Fig. 1. Segmented phantom with 20 tissues and air.

photon). This simplification is widely accepted in the scientific community for significantly reducing simulation time without incurring relevant deviations in the calculations (Sarrut et al., 2014).

GATE provides several navigator algorithms to track the particles from voxel to voxel. The Regular parameterization method allows for fast direct neighboring voxel identification with minimal memory overhead, significantly accelerating the simulation. The Nested parameterization method, directly inherited from the Geant4 toolkit and implemented in GATE since version 6.1, relies on a parametrized approach. It splits the 3D volume along the three principal directions, allowing for logarithmic identification of neighboring voxels. The Regionalized parameterization method utilizes an implicit volume representation called segmented volume, along with a customized segmentation procedure and a distance map, minimizing the number of boundary crossings and enhancing the simulation speed. In this study, the Nested parameterization method was used, as it is the most recommended by GATE developers for its efficiency and ability to handle ultra-large numbers of voxels with optimized geometry navigation.

2.2. PET simulation and image reconstruction

A PET scanner model based on Biograph Vision was previously validated with experimental data by (Peña-Acosta et al., 2024), according to the NEMA NU 2–2018 protocol (National Electrical Manufacturers Association, 2018). This scanner consists of 60800 LSO crystals of size 3.2x3.2 × 20 mm^3 arranged in 80 detector rings. The axial extension of the scanner is 25.6 cm and the detector ring diameter is 88.6 cm. The behavior of the scanner is reproduced through the digitizer chain of GATE taking parameters like the energy resolution (10.1%), the coincidence time window (4.7 ns), the energy window (435–585 keV) and the time resolution (214 ps).

Corrections for randoms, scatter, dead time losses and attenuation, as well as data normalization, are implemented for image reconstruction. To perform attenuation correction an attenuation map is used. It is obtained by an Actor of GATE capable of transforming the phantom materials into attenuation coefficients (in cm^{-1}). The normalization is performed using the component-based method proposed in (Pépin et al., 2011), which requires auxiliary simulations from two different types of sources: a cylindrical volume source and a cylindrical surface source. Then, the PET images are reconstructed by applying the Ordered Subsets Expectation-Maximization (OSEM) algorithm implemented in CASTOR (Merlin et al., 2018) with 8 iterations and 5 subsets. The complete procedure for image reconstruction is summarized in the diagram of Fig. 2.

2.3. Dose calculation

Nowadays the MC method is accepted as the most accurate for modeling radiation transport and conducting dosimetric calculations. However, its requirements of a large number of events in the simulations usually imply excessive computational cost, restricting its application in the clinical routine. Nevertheless, it serves as a crucial tool for assessing the precision and reliability of dose calculations derived from alternative methods.

In clinical practice, the MIRD formalism can be applied, which considers that the dose absorbed in each organ is due to the activity present in said organ plus the contribution due to neighboring organs, according to eq. (1):

$$D_{Target} = \sum_{Source} \widetilde{A}_{Source} \bullet S_{(Target \leftarrow Source)} \quad (1)$$

where D_{Target} is the mean absorbed dose (Gy) delivered to the target organ.

A_{Source} is the total number of nuclear events in the source organs (Bq·s). Clinical practice allows the acquisition of several PET scans and considers the biokinetics of radiopharmaceuticals. In the present work, the time-integrated activity in the source organ over a dose-integration period T_D is calculated with eq. (2). Since 18F has a short physical half-life, T_D is assumed to be infinite.

$$\widetilde{A}_{Source} = \int_0^{T_D} A_{Source}(t)dt \quad (2)$$

S(Target←Source), or S-Value, is the mean absorbed dose to a given target per nuclear disintegration in the source organ, expressed in Gy·Bq^{-1}·s^{-1} (Eq. (3)).

$$S_{(Target \leftarrow Source)} = \sum_i Y_i \bullet E_i \bullet \varphi_{(Target \leftarrow Source)} \quad (3)$$

being Y_i the yield of ionizing radiation type i (Bq^{-1}·s^{-1}), Ei the energy of ionizing radiation type i (J), and $\varphi_{(Target \leftarrow Source)}$ the specific absorbed fraction for ionizing radiation of type i (kg^{-1}). As far as this work, S-Values are calculated as the stored values using the DoseActor of GATE divided by the total histories simulated.

Dose calculations following the MIRD formalism at the voxel level provide more accurate estimates than methods based on compartmental models. However, they also consider a homogeneous distribution of activity in each organ or tissue. In this work, the dose at several organs is also estimated based on a Monte Carlo simulation with GATE and assuming an activity calculated from metabolic images of the patient with whom the voxelized phantom has been built. Thus, activity concentration (Bq/ml) in each voxel at time zero is obtained with eq (4)

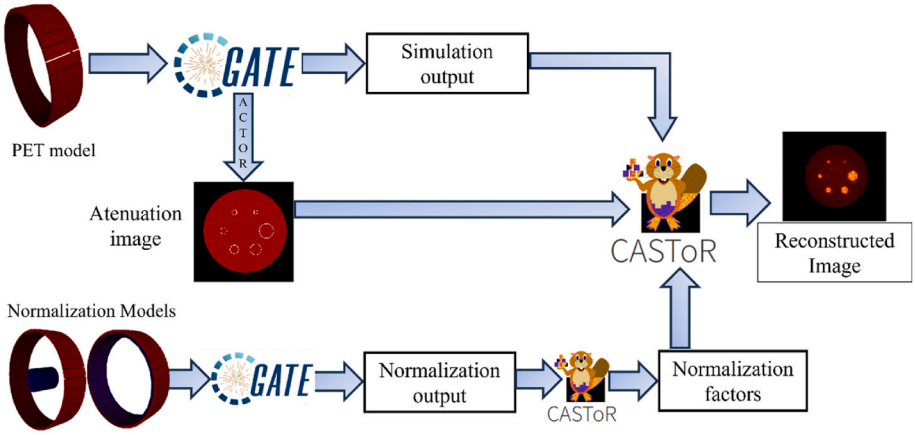

Fig. 2. Image reconstruction diagram using GATE and CASToR.

(Soongsathitanon et al., 2012):

$$Aconc. = Pixel\ Value \bullet Rescale\ Slope + Rescale\ Intercept \quad (4)$$

being the RescaleSlope equal to 1.6545 and RescaleIntercept equal to zero.

Then, the activity per voxel is derived from the activity concentration and the voxel size. If the biokinetics of the 18F FDG is not considered and the decrease in activity is only due to the radiotracer decay, the total accumulated activity (MBq·s) in the phantom is calculated with eq. (2). These events are used to estimate the total dose from the MC simulation, which provides dose per event in every segmented organ.

3. Results and discussion

3.1. Biograph Vision scanner simulation

Fig. 3 displays the outcomes of this simulation, illustrating a cross-section of the pelvic region of the phantom. There, distinct concentrations of radiotracer are discernible within the urinary bladder, enabling the identification of lesions. This is attributed, in part, to the potential of GATE, as well as to the resolution, sensitivity and LSO crystals of the Biograph Vision scanner. In this regard, the easy modeling of architectures with GATE may facilitate the comparison of performance among different technologies, starting from the characteristics of the same phantom. Likewise, to implement improvements in a commercial scanner, modifications in its geometry or materials could be studied.

3.2. S-values and dose calculation

The S-values as described in the Methodology section are based on a Monte Carlo simulation of 2E8 histories, in which the prostate gland acts as a source organ. Table 1 shows some reference values calculated with Opendose (Chauvin et al., 2020) for the ICRP110 phantom and 18F-FDG as radionuclide, and those with GATE for the voxelized phantom built for this work. Relative differences cover a wide range (0.5%–67.9%). In the case of a self-irradiation condition with the prostate, the relative difference of 56.7% is comparable to the results of (Bakkali et al., 2022) (10.74%–86.62% depending on the radionuclide).

On the other hand, dose can be directly calculated with Monte Carlo simulations with GATE. Dose at the segmented organs have been obtained from a source map estimated from metabolic images of the patient. In this case, it was assumed that an injection of 466 MBq for a 104 kg adult male undergoing a prostate PET examination. Based on this premise, the total accumulated activity over an infinite time is 2.98E6 MBqs. Note that this calculation has been done without considering the biokinetics of radiopharmaceuticals. For the prostate gland the dose obtained is 8.1 mGy or 0.07 mGy/MBq. This value is consistent with other recent works found in the literature, in which Karimipourfard et al. (2022) report dose per activity values within 0.02–0.06 mGy/MBq for most organs, and Neira et al. (2020) present as approximate simulation results 6 mGy and 0.025 mGy/MBq in prostate, in PET studies with similar characteristics.

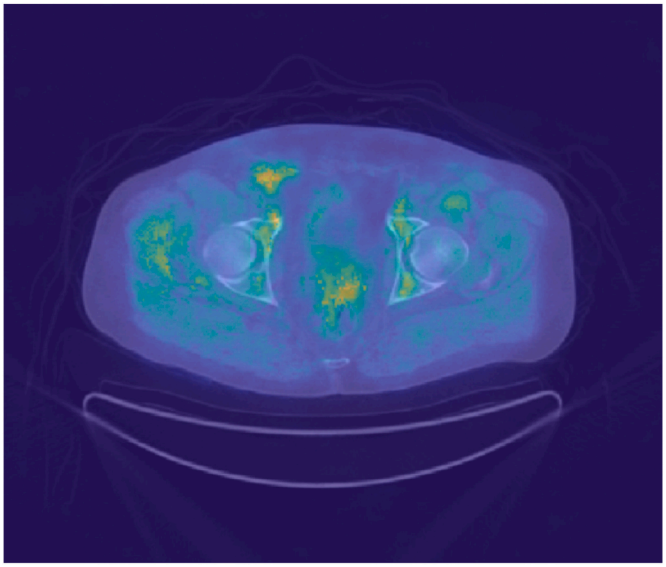

Fig. 3. Reconstructed image merged with the CT image.

Table 1
S-values (mGy/MBq.s) calculated in the prostate gland and its surrounding healthy organs in two voxelized phantoms.

Tissue	ICRP Phantom with Opendose	Patient Phantom with GATE	Relative difference (%)
Prostate	3.29E-04	1.52E-04	−56.7%
Rectum wall	1.76E-05	1.76E-05	−0.5%
Urinary bladder wall	1.73E-05	2.90E-05	67.9%
Pelvis cortical	6.08E-06	3.60E-06	−40.7%
Pelvis spongiosa	5.21E-06	3.60E-06	−30.9%
Sacrum cortical	2.70E-06	1.96E-06	−27.4%
Sacrum spongiosa	2.03E-06	1.47E-06	−27.9%
Femora upper cortical	2.01E-06	1.18E-06	−41.5%
Femora upper spongiosa	2.54E-06	1.24E-06	−50.9%

4. Conclusions

The integration of CT and PET enables the simultaneous acquisition of anatomical and functional information, thereby enhancing diagnostic accuracy and clinical decision-making. The GATE toolkit provides a versatile platform for accurate simulation modeling. A model, incorporating both the CT phantom and activity distribution, was developed, considering the Biograph Vision PET scanner. Coincidence data were reconstructed with CASTOR using the OSEM algorithm. Additionally, a dose actor of GATE was employed to derive the dose distribution at the voxel level corresponding to 466 MBq of 18F-FDG injected activity. The S-Value was calculated for the prostate gland, resulting in a value of 1.52 E−4 mGy/MBq·s, which aligns well with values reported in the literature. Regarding the S-Values in the surrounding organs, relative differences respect to ICRP Phantom with Opendose cover a wide range (0.5%–67.9%). These differences can be attributed to the different phantom considered in the calculation and they are comparable to those of literature with other voxelized phantoms.

CRediT authorship contribution statement

María Lorduy-Alós: Writing – review & editing, Writing – original draft, Supervision, Methodology, Investigation, Conceptualization. **Pedro H. Avelino de Andrade:** Writing – original draft, Software, Methodology, Investigation. **Miriam Magela Peña-Acosta:** Writing – original draft, Software, Investigation, Formal analysis, Methodology. **Sergio Gallardo:** Writing – review & editing, Supervision, Methodology, Investigation, Conceptualization. **Gumersindo Verdú:** Supervision, Project administration, Conceptualization, Funding acquisition.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

The authors are unable or have chosen not to specify which data has been used.

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