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RADIOBIOLOGY, ECOLOGY AND NUCLEAR MEDICINE

Geant4/GATE Comparison of Geometry Optimization Algorithms for Internal Dosimetry Using Voxelized Phantoms

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Abstract—Geant4 Application for Tomographic Emission (GATE) is a Monte Carlo code, including the algorithms integrated inside Geant4 and other specific tools dedicated to tomography. Though, the detailed physical modeling of Geant4 is computationally demanding in order to simulate photon interactions and transport, particularly using voxelized phantoms. To circumvent the relatively slow simulation of voxelized phantoms for radiotherapy applications, GATE offers some relevant optimization methods to minimize the time consumption. In this study, specific absorbed fractions (SAFs) in Golem voxelized phantom using GATE Monte Carlo code for three optimization algorithms: Nested Parametrized Volume, Regular navigation algorithm and Compressed voxels methods have been used to calculate SAFs and compared to the literature data. The computation time has been also compared and discussed for the three methods. Compressed voxels method is more than 16 times faster than the two other parameterization methods for internal dosimetry field.

Keywords: internal dosimetry, Geant4/GATE, voxelized phantoms, parameterization methods

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1. INTRODUCTION

The internal dosimetry estimation, in radiation therapy and nuclear medicine, is highly recommended especially for the therapeutic field. However, to assess the absorbed dose, the specific absorbed fraction (SAF) should be calculated using Monte Carlo simulation. For this purpose, several Monte Carlo codes can be used to estimate radiation dose at the organs, such as Geant4 [1] and its application to Tomography Emission (GATE) [2]. However, all Monte Carlo simulations using a voxelized phantoms extracted from CT images, have a time consuming, especially for high CT resolution and large volumes. In this regard, each Monte Carlo code uses several algorithms to define the voxelized geometry and to reduce the computation time.

For each algorithm, three steps are required to describe a volume. The first one is to define a solid describing the geometric representation of the volume. In the second step, Geant4 uses the Logical Volume concept, associated with the solid, to take into account material information, visualization attributes, secondary particles and production thresholds. The last step is to create a physical volume, representing the spatial position of the logical volume. Typically, the voxel size contained in a CT image is in order of few cubic millimeters. For treatment planning, the definition of a region of interest might ensure the inclusion of many organs. The voxelized phantom Golem contains 122 individual organs and tissues which include all "critical" organs identified by the international commission on radiological protection (ICRP), nearly 2.2 million voxels, in which the position and the atomic composition must be stored in memory for each voxel [3]. Loading each voxel into memory requires suitable navigation algorithm. The voxel navigation could affect the simulation efficiency and time computation of GATE/Geant4, especially when using a big geometry. Therefore, several efficient navigation algorithms are developed in Geant4. Also, GATE, based on Geant4, provides various navigation optimization algorithms. For tracking particle inside voxelized phantoms, Geant4 offers three principal algorithms: G4VPVParameterised, G4VNestedParameterisation, and G4PhantomParameterisation classes [4]. Another method was developed by D. Sarrut named Regionalized parameterization method [5].

The purpose of our work is to find out which one of the optimization algorithms introduced in GATE is appropriate for internal dosimetry calculation. Therefore, we will firstly calculate the specific absorbed fractions (SAFs) using the three tracking algorithms: Nested Parametrized Volume, Regular navigation algorithm and Compressed voxels, and compare the results with [6]. Then, we will evaluate the time computing between the three different particle tracking

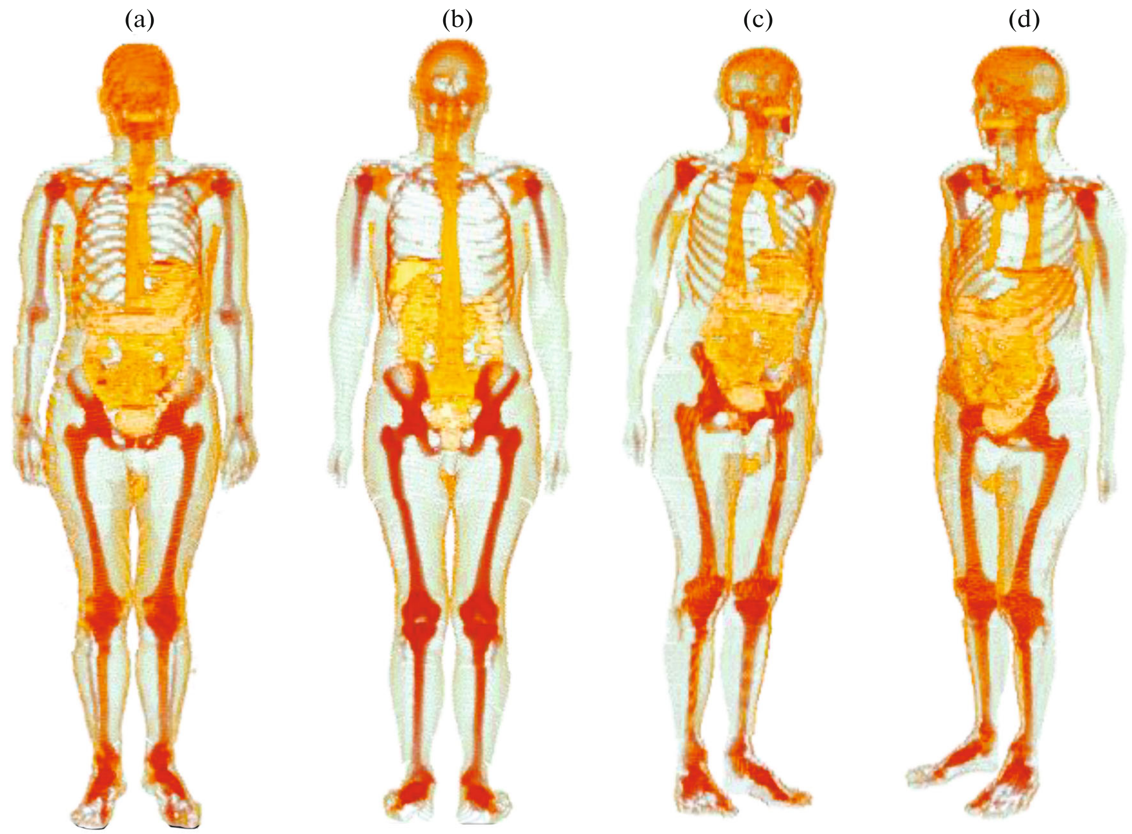

Fig. 1. Golem 3D whole-body views showing (a) anterior; (b) posterior; (c) right side; (d) left side.

algorithms to deduce the fastest one for internal dosimetry.

Some studies [7, 8] have been conducted using GATE optimization algorithms for Positron Emission Tomography (PET). H. Lin et al. [7] developed, for imaging applications in nuclear medicine, a multiple photon emission history generator (MPHG) based on SimSET/PHG. They found out that GATE/MPHG is faster compared to the other GATE/Geant4 particle tracking algorithms. N.S Rehfeld et al. [8] proposed two methods to reduce the time spent on tracking particles in voxelized phantoms, using GATE, for PET simulation; "regular navigation algorithm" of Geant4 and fictitious interaction tracking (also known as Woodcock tracking) for photons. Our paper concerns the internal dosimetry calculation. When the dosimetry calculation is of interest, some simulation parameters (charged particles cuts, sources type, chosen electromagnetic interactions, ...) can be different compared to the PET coincidences simulation, a wrong choice may alter the simulation results.

In the present study, specific absorbed fractions (SAFs) have been calculated using three optimization algorithms inserted in GATE (Nested Parametrized Volume, Regular navigation algorithm and Compressed voxels methods) and compared with the Zankl ones [6] using Golem voxelized phantom. For those three methods, the computation time has been also discussed.

2. MATERIALS AND METHODS

2.1. Golem Voxelized Phantom

Golem voxelized phantom was extracted by the approach suggested by Zankl et al. by exploiting 220 clinical tomographic images of a 38 years living individual with external dimensions close to those of the ICRP Reference Man; 176 cm in tallness and 68.9 kg in weight Fig. 1. A slice is set of pixels that could be represented as a matrix of order 256 × 256. The spatial resolution is $2.08 \times 2.08 \times 8$ mm^3 [3]. The geometry was changed from 8 to 16 bit unsigned integer and to interfile format for usage into GATE.

2.2. Simulation Description

Simulations were carried out for photons from 10 to 4 000 keV. In each simulation, photoelectric absorption, Compton scattering, and pair production were used as the principal radiation interaction processes. Each simulation produces 100 million photons. Timing information was recorded as the total CPU time,

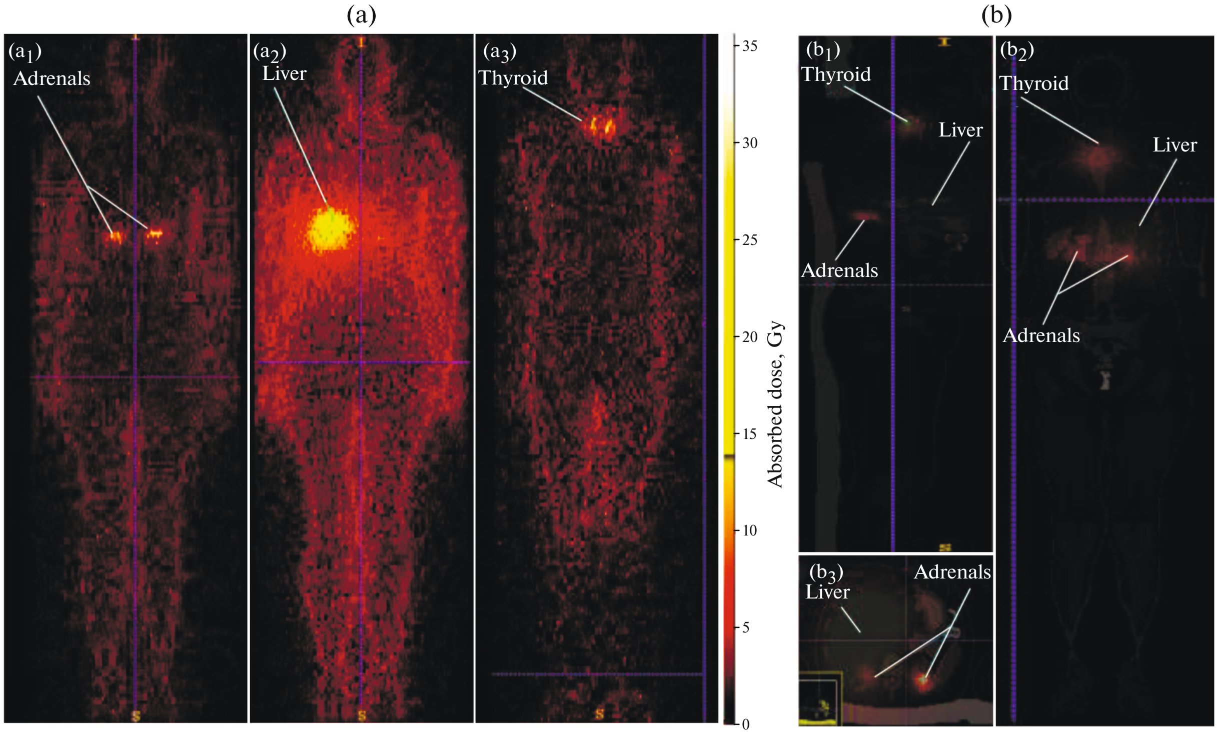

Fig. 2. (a) The dose distribution on Golem Voxelized phantom using Adrenals (a_1), Liver (a_2) and Thyroid (a_3) organ sources. (b) sagittal views (b_1); Coronal views (b_2); and axial views (b_3) of the three selected organ sources used in this paper.

which includes both particle transport time and initialization time. The time computation was recorded using Simulation Statistic Actor inserted in GATE. Each simulation was submitted as an isolated task to the local computing cluster. The Monte Carlo simulations were performed on a node with 20 Intel-Xeon-X5690 CPU with 3.47 GHz, 20 GB of cache and 11.6 GB of RAM. Each job was run on a distinct computing node.

The output file created by GATE gave the deposit energy per voxel of the phantom. Afterward, the deposit of energy was changed over into specific absorbed fraction (SAF). In this study we are using standard physic package lists 3 and the used cut was 0.1 mm for photons and 2 µm for electrons as recommended by [9] for internal dose calculations.

The absorbed fraction ($AF_{(target \leftarrow source)}$) is defined as the fraction of the emitted energy from a given source organ that is absorbed by a given target organ. The specific absorbed fraction (1/kg) is obtained as follow:

$$SAF_{(target \leftarrow source)} = \frac{AF_{(target \leftarrow source)}}{m}, \qquad (1)$$

where, "m" is the target organ mass in kg.

The SAF, specifies the fraction of the energy deposited in the source organ itself and in other target organs. GATE stores the absorbed dose D_i in a given voxel in a 3D matrix Fig. 2, according to the following formula:

$$D_j\,[\mathrm{Gy}] = \frac{E_{\mathrm{dep}}\,[\mathrm{J}]}{\rho\left[\frac{\mathrm{kg}}{\mathrm{cm}^3}\right] \times V\,[\mathrm{cm}^3]}, \qquad (2)$$

where E_{dep} is the energy deposited in the given volume, ρ is the density and V is the voxel volume.

2.3. Voxelized Geometry Description in GATE

Appropriate methods are needed to describe multiple copies of small volume inside a mother volume to implement voxelized patient geometry in GATE. The tracking algorithm and the geometry size influences mainly the calculation time.

The parameterization methods obtained from Geant4 navigation algorithms are generally created in order to economize the memory utilization and the calculation time, using voxelized phantoms. Nested Parametrized Volume, Compressed voxels and Regular navigation algorithm methods are used in our simulation to confront efficiency and computation time between these tracking algorithms, with an aim to optimize GATE in internal dosimetry field. The present work was performed with version 7.1 of the GATE Monte Carlo platform. This version of GATE makes use of Geant4 version 10.01.p01.

2.4. Step Size around the Voxel Boundary

GATE introduces some limitations of the step size: Minimal, UseSafety and UseDistanceToBoundary. Recently a new option, called fUseSaftyPlus, has been implemented in Geant4 since Geant4 version 10.01. When UseDistanceToBoundary mode is employed, a high precision is added to improve simulation near the boundary. The step size becomes equivalent or smaller than the free mean elastic scattering path in a thin region around this boundary. Nevertheless, the step size decreases near the boundary which increases the calculation time. In this study, UseDistanceToBoundary has been chosen for tracking the secondary charged particles, in order to increase the accuracy of the simulation in a small region near the boundary [9].

2.5. Regular Navigation Algorithm

A new navigation algorithm, named regular navigation, was added in GATE 6th version. It can be used for the tracking of particles in voxelized phantoms. A regular navigation algorithm is a generic volume representing a collection of repeated volumes; each copy may be different in size, shape, materials or position. In case of voxelized phantoms extracted from CT images, all voxels have the same dimension, and the geometry is selected by CT slices. For each slice, a vector is created containing the copy number of each voxel and the atomic composition. When a particle enters inside a parameterized volume, the algorithm considers the slice number and the copy number of the voxel in the vector associated with the slice. When a particle arrives at the boundary of a voxel, a new voxel is sought-after in the vector of the current slice or in the neighboring slices. Moreover, in order to limit the time of this search, the algorithm looks at only the six neighbors of the current voxel. However, although there are no limits on the number of voxels, the computation time increases as their number increases because the particles are delayed at each boundary encountered. Regular navigation algorithm includes a new method called ComputeStepSkippingEqualMaterials, when a boundary is confronted, the navigator should search and enter in the following voxel and check if his material is the same as the current one. If it is true, this method is directly called again. Otherwise, new navigator manager will be called which loads the new properties of the next voxel. However, in regular navigation method no daughter volume can be added in a parameterized volume [8].

2.6. Nested Parameterization Method

Another method has been introduced by Geant4 collaboration since version 8.1 [10], using the volume parameterization mechanism and has been included in GATE version 6.1. Nested parameterization method gives GATE opportunity to store a single voxel representation in memory and dynamically changing its position and typesetting at run-time over the navigation. The principal advantage of this strategy is high effectiveness in memory space. Geometry has three-dimensional regular reputation of same volume's character in Nested Parametrized Volume method. Instead of direct three-dimensional parameterized volume, Nested Parametrized Volume uses two replications along two axes and then use one-dimensional parameterization following the third axis. This principle of representation of volumes requires less memory because the material of voxels is characterized by both: its copy number and the duplicate number of its container [11].

2.7. Compressed Voxels Method

As voxelized phantom resolution increases, the number of voxels can turn out to be enormous and a considerable quantity of memory might be required. For most applications in any case, high determination is not required wherever in the phantom but rather just where important to keep smooth boundaries between volume structures. The compressed voxels method can be used to produce a compressed phantom where voxel size is variable. With the compression algorithm, all neighboring voxels of a similar material are combined to make the biggest conceivable rectangular voxel. A compressed phantom utilizes less memory and furthermore less CPU [12].

2.8. Data Analysis

The ratio (R) between SAF values derived from GATE/GEANT (SAF_{GATE}) and the corresponding reference values ($SAF_{reference}$) for each photon energy was calculated as:

$$R = \frac{SAF_{GATE}}{SAF_{reference}}.$$

The SAF's compressed voxels method (CM) has been chosen as reference for the three optimization algorithms comparison. In addition, the Zankl SAFs have been used as reference to compare between GATE results and the literature. The relative difference (RD %) can be obtained as follow:

$$RD\% = |1 - R| \times 100.$$

3. RESULTS AND DISCUSSION

3.1. SAFs Calculation Using Various GATE Optimization Algorithms

In this study, SAFs have been calculated using GATE Monte Carlo code using various optimization algorithms: Nested Parametrized Volume, Regular navigation algorithm and Compressed voxels methods, for energy photons between 10 and 4000 keV as

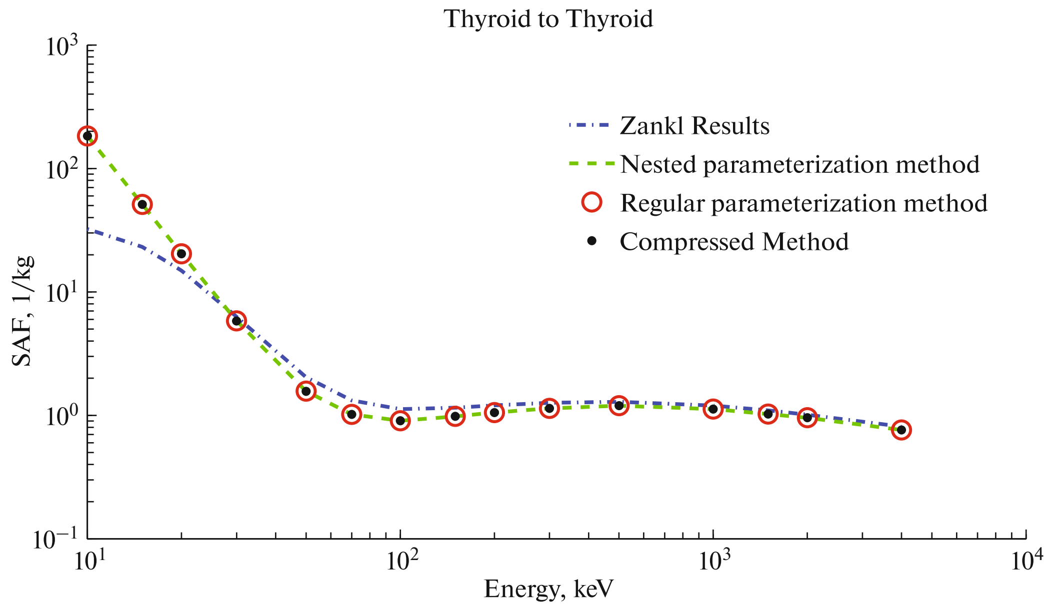

Fig. 3. Graphic representation of calculated thyroid-to-thyroid self-absorption fractions with GATE and GSF Monte Carlo codes corresponding to the Golem adult male phantom.

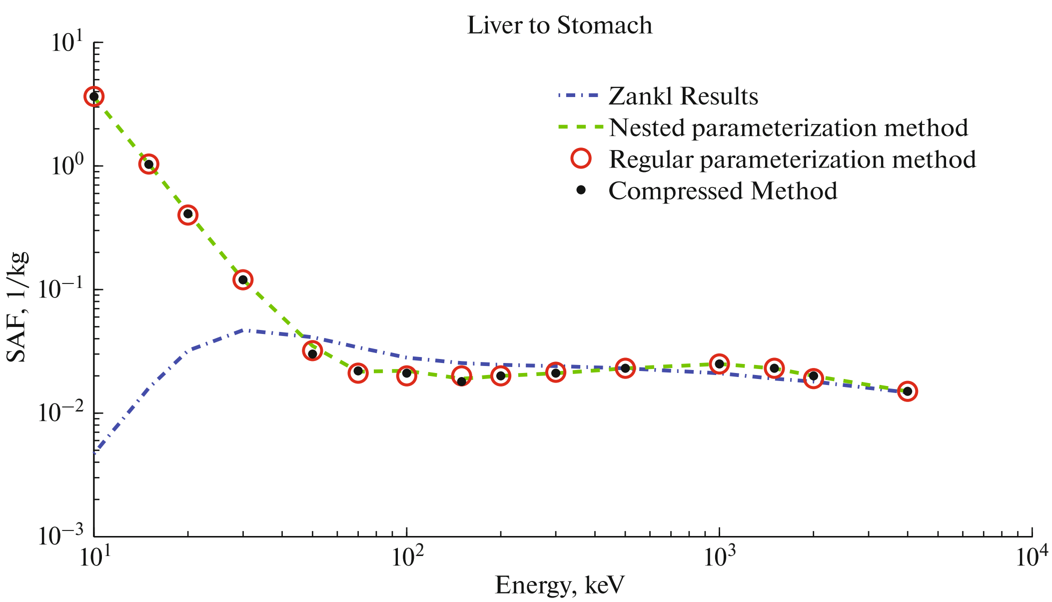

Fig. 4. SAFs using GATE for different voxelization algorithms and GSF Monte Carlo code for liver source organ to stomach target organ.

shown in Figs. 3–5. The R ratios, corresponding to CM reference values, were within 1.000 ± 0.001 for self-absorption (Table 1). That means that there is basically no difference between these three methods regarding the SAFs calculation for self absorption. For cross irradiation to other organs, the ratios between two series of results were in the range of 1.000 ± 0.050 except photon energies of 50 keV (Table 2), 100 and 200 keV (Table 3), where the ratios are 1.17, 1.07, 1.10, and 1.20 respectively.

3.2. Comparison between GATE and Zankl Results

3.2.1. Self-absorption. As mentioned above, we have calculated SAFs, corresponding to photonic energies between 10 and 4000 keV, in the case where the thyroid represents both the source and the target organs, i.e. the self-absorption. The SAFs values obtained by GATE with Nested, Regular Parameterization and Compressed voxels methods are compared to Zankl's results [6], as shown in Fig. 3.

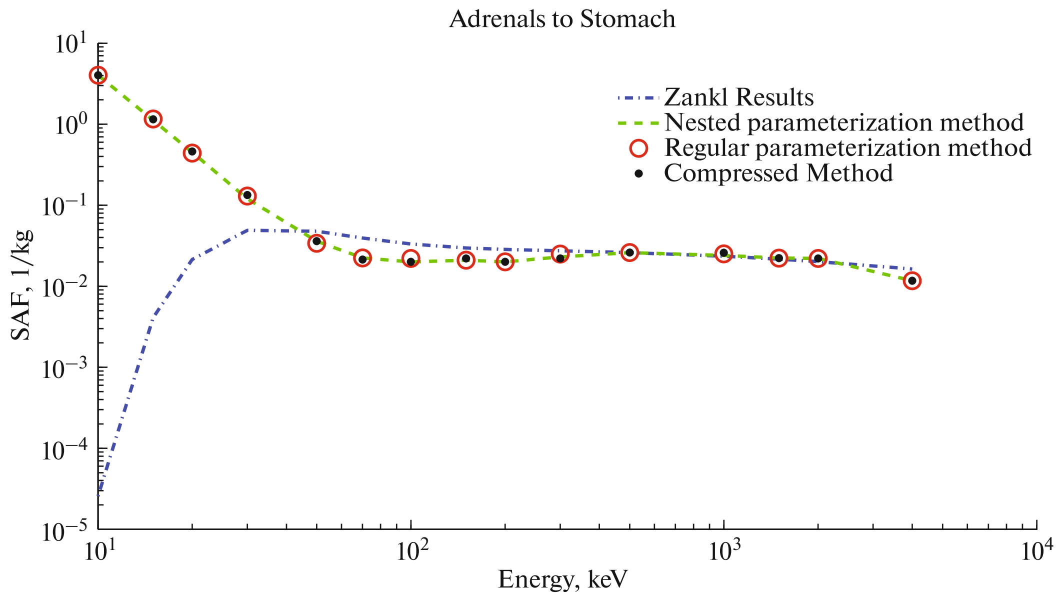

Fig. 5. SAFs using GATE for different voxelization algorithms and GSF Monte Carlo code for adrenals source organs to stomach.

For energy less than 30 keV, the largest discrepancy between GATE and Zankl results was high (more than 100%). As far as photon energy between 30 and 300 keV the largest relative difference was 23.1% Table 1. This considerable disagreement between Zankl and GATE for low energy might be due to the difference between the physic lists used by Gate and GSF Monte Carlo codes. Indeed, Geant4 standard physic lists—used in this case—were created for high energy photons. These disparities for low energy confirm some results already shown by [13, 14] which indicate that there is weak agreement for low energy, between the Geant4/GATE results and the other published data including EGS and MIRD. Concerning high energy—

Table 1. Calculated SAFs$_{(\text{thyroid} \leftarrow \text{thyroid})}$ (1/kg) for three voxelization algorithms using GATE, compared with Zankl results [7], for photons energy from 10 to 4000 keV. The Nested Parametrized Volume and Regular navigation algorithms are compared to the compressed voxels method

Energy, keV	Zankl	Nested	Regular	Compressed voxels (CM)	CM/Zankl	Nested/CM	Regular/CM
10	32.320	183.340	183.320	183.360	5.673	1.000	1.000
15	23.140	51.130	51.129	51.130	2.210	1.000	1.000
20	14.910	20.353	20.352	20.353	1.365	1.000	1.000
30	6.288	5.827	5.827	5.820	0.926	1.001	1.001
50	2.037	1.571	1.571	1.571	0.771	1.000	1.000
70	1.322	1.018	1.017	1.017	0.769	1.001	1.000
100	1.123	0.906	0.906	0.905	0.806	1.001	1.001
150	1.153	0.980	0.979	0.980	0.850	1.000	0.999
200	1.205	1.055	1.056	1.056	0.876	0.999	1.000
300	1.265	1.138	1.138	1.139	0.900	0.999	0.999
500	1.288	1.197	1.197	1.196	0.929	1.001	1.001
1000	1.200	1.124	1.124	1.124	0.937	1.000	1.000
1500	1.097	1.024	1.025	1.025	0.934	0.999	1.000
2000	1.012	0.957	0.957	0.957	0.946	1.000	1.000
4000	0.810	0.782	0.782	0.781	0.964	1.001	1.001

Table 2. Calculated SAFs$_{(\text{stomach wall} \leftarrow \text{liver})}$ (1/kg) for three voxelization algorithms using GATE, compared with Zankl results [7], for photons energy from 10 to 4000 keV. The Nested Parametrized Volume and Regular navigation algorithms are compared to the compressed voxels method

Energy, keV	Zankl	Nested	Regular	Compressed voxels (CM)	CM/Zankl	Nested/CM	Regular/CM
10	0.004	3.600	3.660	3.650	–	0.986	1.003
15	0.016	1.035	1.036	1.030	–	1.005	1.006
20	0.032	0.420	0.400	0.410	12.813	1.024	0.976
30	0.047	0.120	0.120	0.120	2.553	1.000	1.000
50	0.041	0.035	0.032	0.030	0.732	1.167	1.067
70	0.029	0.021	0.021	0.021	0.724	1.000	1.000
100	0.028	0.022	0.022	0.021	0.750	1.048	1.048
150	0.025	0.020	0.020	0.020	0.800	1.000	1.000
200	0.024	0.022	0.022	0.022	0.917	1.000	1.000
300	0.024	0.021	0.021	0.021	0.875	1.000	1.000
500	0.023	0.023	0.023	0.023	1.000	1.000	1.000
1000	0.022	0.025	0.025	0.025	1.136	1.000	1.000
1500	0.021	0.023	0.023	0.023	1.095	1.000	1.000
2000	0.018	0.020	0.020	0.020	1.111	1.000	1.000
4000	0.015	0.015	0.015	0.015	1.020	1.000	1.000

Table 3. Calculated SAFs$_{(\text{stomach wall} \leftarrow \text{adrenals})}$ (1/kg) for three voxelization algorithms using GATE, compared with Zankl results [7], for photons energy from 10 to 4000 keV. The Nested and Regular navigation algorithms are compared to the compressed voxels method

Energy, keV	Zankl	Nested	Regular	Compressed voxels(CM)	CM/Zankl	Nested/CM	Regular/CM
10	–	4.031	4.032	4.030	–	1.000	1.000
15	0.004	1.120	1.160	1.150	–	0.974	1.009
20	0.021	0.450	0.460	0.460	21.905	0.978	1.000
30	0.049	0.130	0.130	0.131	2.673	0.992	0.992
50	0.048	0.036	0.036	0.036	0.750	1.000	1.000
70	0.029	0.022	0.022	0.022	0.759	1.000	1.000
100	0.028	0.020	0.022	0.020	0.714	1.000	1.100
150	0.028	0.021	0.021	0.021	0.750	1.000	1.000
200	0.026	0.024	0.020	0.020	0.769	1.200	1.000
300	0.025	0.023	0.023	0.023	0.920	1.000	1.000
500	0.024	0.026	0.026	0.027	1.125	0.963	0.963
1000	0.025	0.027	0.027	0.027	1.080	1.000	1.000
1500	0.022	0.022	0.022	0.022	1.000	1.000	1.000
2000	0.020	0.022	0.022	0.022	1.100	1.000	1.000
4000	0.016	0.017	0.017	0.017	1.063	1.000	1.000

more than 300 keV – the outcomes between Zankl and Gate were practically similar as shown in Fig. 3. The largest relative difference was 7.1% (Table 1).

3.2.2. Cross irradiation to other organs. SAFs calculated by Nested Parametrized Volume, Regular navigation algorithm and Compressed voxels methods have been computed using GATE Monte Carlo code for photons energy between 10 and 4000 keV, in the case where the stomach is the target organ and the liver or adrenals are the source organs as shown in Figs. 4 and 5. Our results show that there is an acceptable agreement with relative difference around 10%, between Zankl and Gate for the energy more than 300 keV. For energy between 50 and 300 keV, the rela-

Table 4. Memory consumption for three voxelization algorithms using Thyroid, Liver and Adrenals as source organs

Geometry type	Source and target organs (source → target)	Minimum memory, KB	Maximum memory, KB	Average memory, KB
Nested parametrized volume	Thyroid → Thyroid	325.0	327.3	325.6
	Liver → Stomach wall	337.3	339.8	338.7
	Adrenals → Stomach wall	325.7	328.1	326.5
Regular navigation algorithm	Thyroid → Thyroid	431.4	433.2	432.5
	Liver → Stomach wall	442.8	444.6	443.9
	Adrenals → Stomach wall	430.9	432.8	431.7
Compressed voxels	Thyroid → Thyroid	265.9	267.9	266.3
	Liver → Stomach wall	277.8	279.8	278.3
	Adrenals → Stomach wall	265.9	268.2	267.5

tive difference was about 25% for photons emitted by liver and adrenals as shown in the Tables 2, 3. Concerning low energy less than 50 keV, the relative difference was more than 100%. The main reasons of these disparities were already discussed in the previous paragraph.

3.3. Memory Consumption

Table 4 presents the memory consumption in the case of three different sources (Thyroid, Liver and Adrenals), two different targets (Thyroid and Stomach wall) and for the three tracking optimization algorithms. Regardless the organ source, "compressed voxels method" consumes less memory compared to Nested Parametrized Volume and Regular navigation algorithm, with a relative difference of 22 and 60% respectively. Furthermore, Nested Parametrized Volume uses less memory consumption than Regular navigation algorithm.

3.4. Timing

The speed of the three methods was determined with the same patient geometry, physic lists, computer hardware and primary particles. Figures 6–8 show that there is no big difference between calculation time for Nested Parametrized Volume and Regular navigation algorithm. However, there is a big time disparity between those two parameterization methods and compressed voxels method. Indeed, the compressed voxels method was more than 16 times faster than the two other parameterization methods; Nested Parametrized Volume and Regular navigation methods. Employing the compression algorithm, all adjacent voxels of the same material are fused together to form the largest possible rectangular voxel. In this case, a compressed phantom uses less memory (Table 4), less CPU and less computing time. That means that in case of dose calculation with voxelized phantoms the compressed voxels method is much faster and gives practically the same results with a relative difference less than 5% in comparison with the other GATE parameterization methods, except photon energies of 50 keV (Table 2), 100 and 200 keV (Table 3), where the relative differences are 16.7, 6.7, 10 and 20% respectively.

H. Lin et al. [7] and N.S. Rehfeld et al. [8] find that regular navigation method is faster than compressed voxels method when tracking only photons particles, without secondary charged particles, in PET simulation. According to N.S. Rehfeld et al. [8], regular navigation method is 2 to 5 times faster than compressed voxels, depending on the phantom voxels number, for imaging simulation field. However, in dosimetry applications (SAF calculation) the secondary charged particles must be tracked. And the performance of the results is limited by the electron range cut in the phantom. In fact, concerning dosimetry applications, N.S. Rehfeld et al. recommend to adjust the electron cut to the required accuracy.

With regard to H. Lin et al. [7], the GATE/MPHG is the fastest method using Micro PET scanner. This method, where cut-offs are set to 500 mm, ignores the simulation of electrons. This cut is sufficiently large to suppress the production of electrons in the phantom. In fact, such as method can be useful for simulations of imaging applications in nuclear medicine, but once charged particle simulations are required, e.g. for dosimetry applications, H. Lin et al. recommend the other particle tracking methods such as compressed voxels [7], with careful verification of the transportation step size.

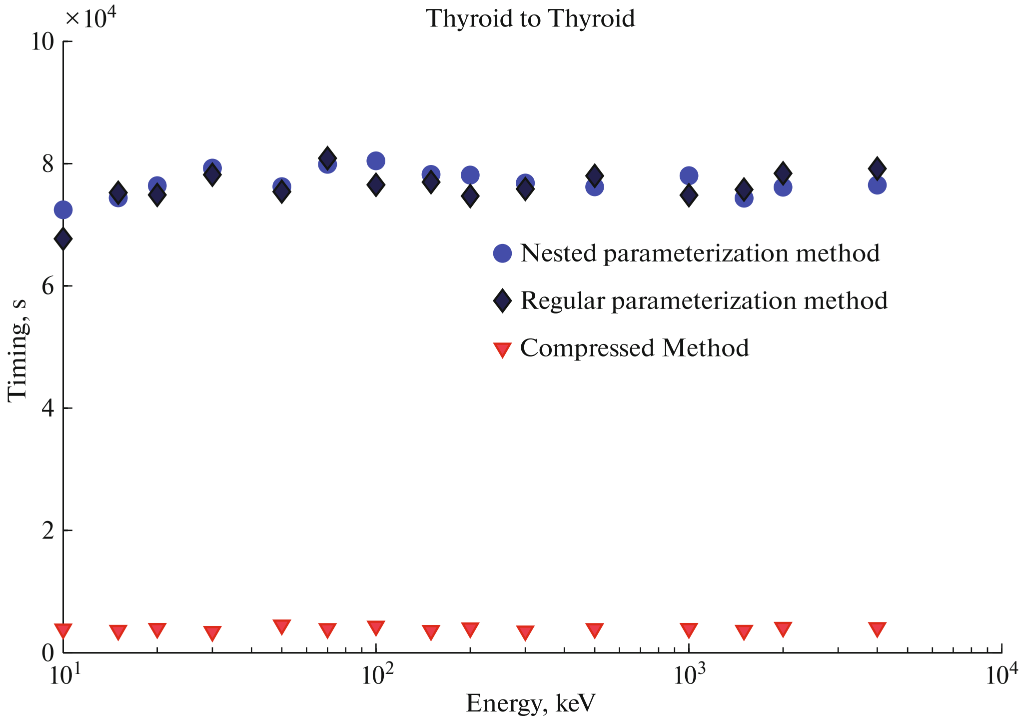

Fig. 6. Computation time comparison between different voxelization algorithms for thyroid as source and target organ using GATE.

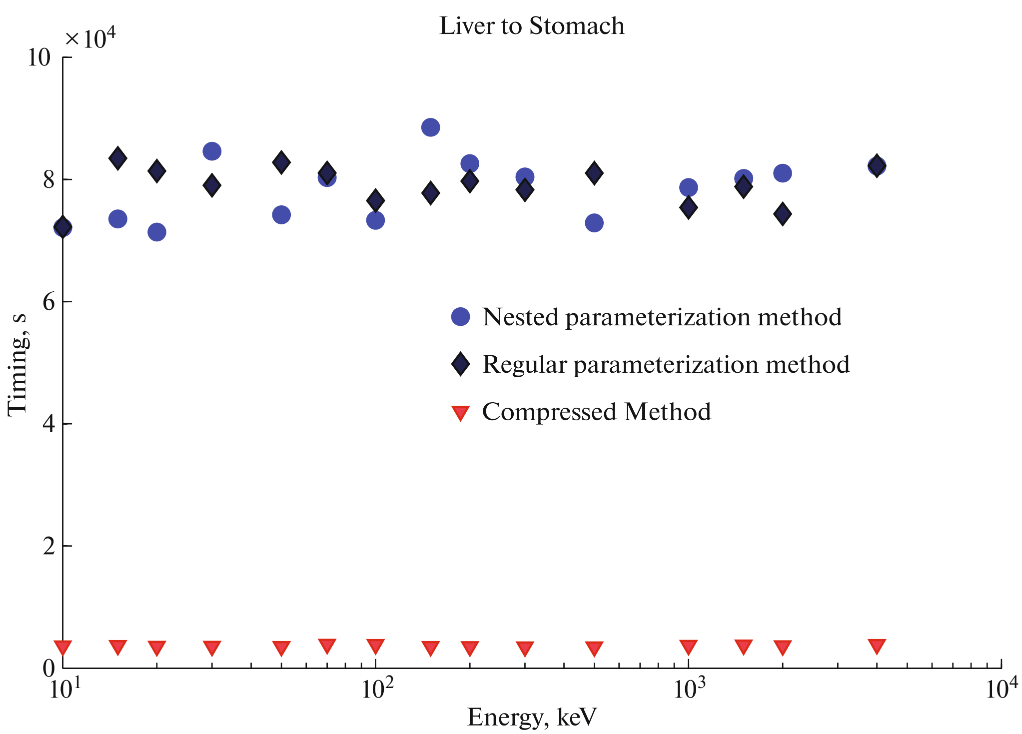

Fig. 7. Computation time comparison between different voxelization algorithms for liver source organ to stomach using GATE.

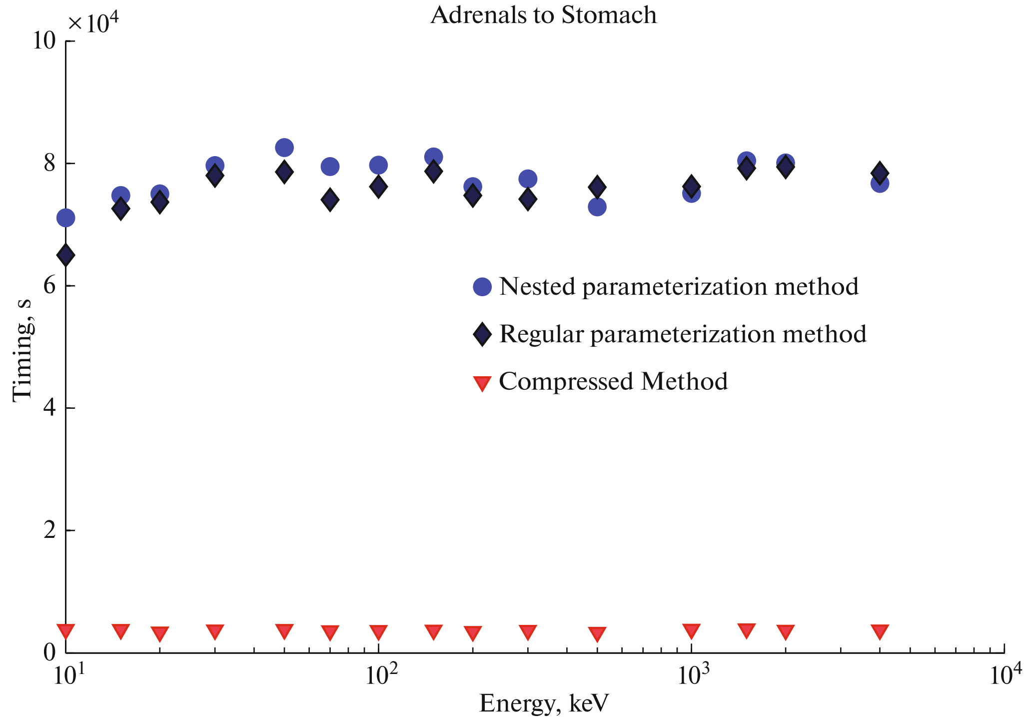

Fig. 8. Computation time comparison between different voxelization algorithms for adrenals source organs to stomach using GATE.

Indeed, simulation of imaging applications with PET scanner is dissimilar to dosimetric simulation, especially with various geometry and transportation step size. Whereas the speed up of the simulation is related to the geometry complexity, the particles type, the step size and the number of different materials used, so the speed up may not be similar between imaging and dosimetric simulation.

In addition, the ion and back-to-back sources, used for PET by [7, 8] respectively, are different. These different source options may represent a disagreement in terms of computing time, when tracking particles in GATE. In a future work, we will discuss widely the parameters that can affect the computation time when tracking particles through voxelized phantom using GATE for both; imagery simulation and dosimetry calculation.

4. CONCLUSIONS

The obtained results show good agreement with Zankl's one for energy equal or greater than 300 keV. For lower energy the difference was relatively higher between GATE and Zankl results. This difference increases when the energy decreases. Concerning GATE computing time, there is no big difference between Nested Parametrized Volume and Regular navigation algorithm. However, there is big CPU time difference between those two parameterization methods and compressed voxels method. Although the compressed voxels method is much faster, it also gives the same results with low disagreement compared to the other parameterization methods for dose calculation.

The compressed voxels method reduces the number of material boundaries enough and allows us to decrease computational time by a factor up to 16, while keeping memory consumption low. Eventually, this study shows that such a method is considered suitable for internal dosimetry as recommended by [7, 12].

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