GATE Monte Carlo simulation toolkit for medical physics

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Abstract. The GATE toolkit (GEANT4 Application for Tomographic Emission) is a GEANT4-based (GEometry ANd Tracking) platform for Monte Carlo simulations in medical physics. GATE applications can be divided into two main axes: radiation-based medical imaging and radiotherapy/dosimetry. The accurate modeling of the first one is crucial for system design and optimization as well as for development and refinement of image analysis algorithms. The

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importance of the precise simulation of the second is essential for characterisation of external beam radiotherapy (proton therapy and carbon ion therapy) and absorbed dose assessment. Within this paper, we discuss the main features of GATE and give a general view on applications, followed by insights into future development perspectives.

1 Introduction

The GATE Monte Carlo toolkit (GEANT4 Application for Tomographic Emission)[1–3] is GEANT4 (GEometry ANd Tracking) [4] based platform for numerical simulations in medical imaging and radiotherapy. GEANT4 is a platform for the Monte Carlo simulation of the passage of elementary particles through matter developed for high energy physics and nuclear experiments, accelerator and space physics studies. Utilizing GEANT4's core engine, GATE simplifies complex simulations through a user-friendly macro language and provides opportunity for medical physics simulations. GATE aligns with the evolving GEANT4 toolkit, releasing a new version annually, synchronized with the latest GEANT4 release. Both of platforms are open source and based on C++.

The GATE code is managed by OpenGATE scientific collaboration, comprised of 25 institutions (www.opengatecollaboration.org). It is dedicated to the development, maintenance, and promotion of the GATE software. Governed by a Gentleman's agreement, the collaboration welcomes contributions and operates under the guidance of a spokesperson and scientific coordinator. Biannual workshops facilitate discussions on current developments, validations, and priorities, while a group of developers regularly addresses technical challenges, open to all contributors.

GATE is one among several other Monte Carlo codes (GEANT4 itself, MCNP [5], GAMOS [6], TOPAS [7]) which are in use in medical physics applications. The collaborative and open source approach is a feature of GATE providing both advantages such as broad and powerful feature enrichment and limitations such as code coherence and efficiency.

The source code is stored in Git repositories within the GitHub organization named OpenGATE, comprising four main repositories, namely `Gate` (housing the main source code), `GateBenchmarks` collecting benchmarks, `GateContrib` collecting users' contribution examples, and `GateTools` offering additional Python tools.

Typical GATE applications are generally split into two sub-domains: imaging and dosimetry for radiotherapy. The first one includes simulation of radiation-based imaging systems such as: Positron Emission Tomography (PET), Single Photon Emission Tomography (SPECT), Compton Camera, Computed Tomography (CT), CBCT (Cone-Beam CT), etc. Such types of simulation represent a keystone to design or improve imaging systems, to optimize acquisition parameters, and to develop advanced image processing algorithms. The second domain refers to several types of radiation therapies such as external beam radiotherapy (including proton and carbon ion therapy). This also concerns absorbed dose assessment and energy deposition in imaging, such as CT or interventional radiology.

Wide number of users' application can be illustrated by figure 1 depicting an estimation of the number of publications throughout the lifetime of GATE, covering all the available applications in medical physics (with almost 900 publications from 2004 until 2021). Figure 2 summarizes the main applications of GATE that can be found in the literature, also separated into two main fields, imaging and dosimetry.

In this paper, we present the main features of GATE and give a general view on imaging and radiotherapy applications. It is also followed by future development perspectives.

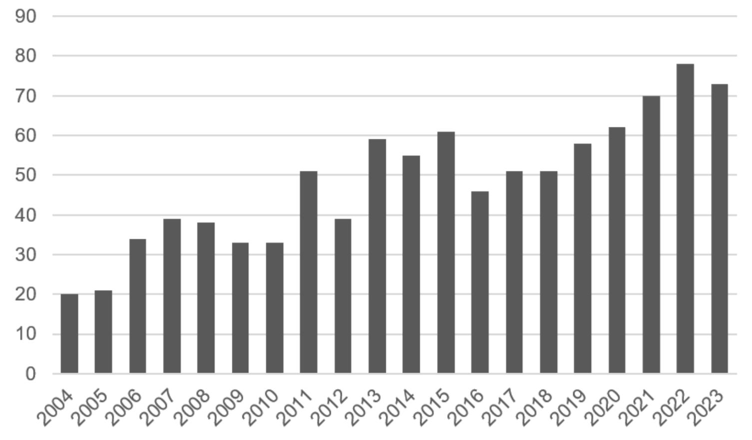

Figure 1. Estimated number of publications of GATE from 2004 to 2023 regarding imaging, dosimetry and radiotherapy applications. The graph is provided by the Scopus platform (www.scopus.com)

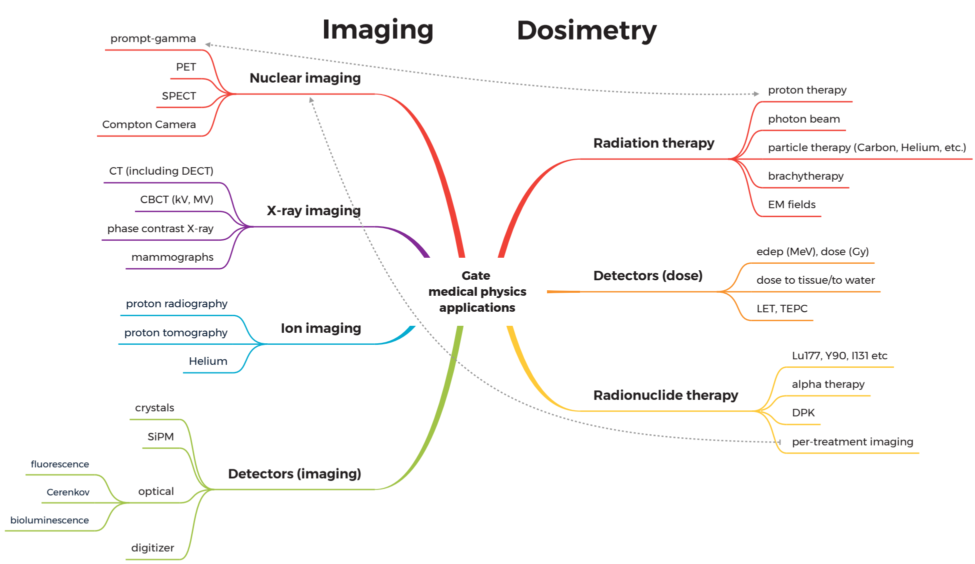

Figure 2. Main applications of GATE in medical physics.

2 GATE and its medical physics applications

2.1 Some aspects of GATE architecture

GATE effectively combines the strengths of the GEANT4 simulation toolkit, integrating well-validated physics models, advanced geometry description and robust visualization tools.Comprising several hundred C++ classes, GATE architecture can be represented by three layers on the top of GEANT4 (figure 3): Core, Application and User. The Core layer manages time, geometry, and radioactive sources, aligning closely with the GEANT4 kernel. The Application layer allows users to implement classes derived from the Core layer, enabling the creation of specific geometrical volume shapes and operations like rotations or translations. On top of the Application layer is the User layer, where end-users can simulate experiments using an extended version of the GEANT4 scripting language without knowledge in C++ programming. GATE employs a dedicated scripting mechanism, referred to as the macro language, extending GEANT4's native command interpreter to execute and control Monte Carlo simulations effortlessly. One notable feature of GATE is its ability to synchronize time-dependent components for a coherent acquisition process description. Additionally, GATE facilitates realistic modeling of detector output by incorporating GEANT4 interaction histories, allowing users to mimic detector electronic response, including cross-talk, energy resolution, and trigger efficiency, through a user-defined linear processing chain (see *Digitizer Unit* below).

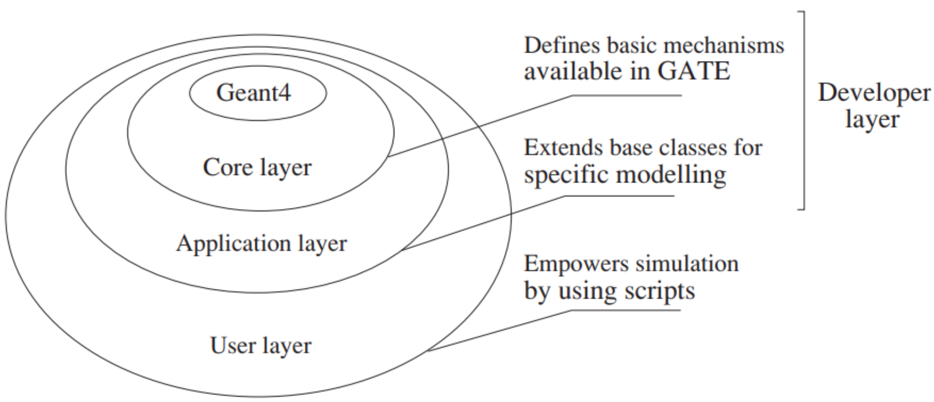

Figure 3. Sketch of the layered architecture of GATE [1].

We also would like to focus on three three key concept of the GATE architecture which are "Volumes" the handling of the geometry, "Actors" that serve several scoring purposes, and the "Digitizer Unit" specific for imaging systems.

Volumes

In GEANT4, all geometrical elements that compose a simulation are described with three concepts. `LogicalVolume`s represent the properties (e.g. material composition), `PhysicalVolume`s manage the spatial positioning, and `Solids` define the shape of a geometrical element. In GATE, the three concepts are encapsulated into a single `GateVolume` that abstracts those notions. The user only manipulates *Volumes* without the burden to manage the three different concepts.

Actors

The Actors are scorers that encapsulate several GEANT4 concepts. They are used as a callback from the GEANT4 engine to score information or modify the default behavior of particles during a simulation. An Actor combines the GEANT4 `SensitiveDetector` and `Actions` callbacks within a single class that can perform tasks each time a Run, Event, Track or Step starts or ends in a given volume. Actors are mainly used to record parameters or information of interest calculated during the simulation, but they can also be used to act on the current particle, for example to stop tracking it. It is also possible to associate each Actor with one or more filters allowing to select a type of particle, an energy or even a specific direction. About 30 Actors are currently available.

Digitizer Unit

The photodetection component response in PET, SPECT, or Compton Camera detector modeling is handled by a suite of analytical and semi-analytical models forming a *Digitizer Unit*. This module is based on GEANT4 virtual methods dedicated for such functionality. It takes as input a list of interaction events within a crystal or detector element and generates digital pulses or *Digis* with associated information (energy, position, time, etc). The first step of digitization in GATE is to construct *Single* digits, each of them mimics one specific hardware response with their associated uncertainty. In the case of PET imaging, a specific Digitizer Unit part for constructing coincidences exists.

2.2 Imaging applications

Nuclear medicine imaging

Over the past few decades, imaging modalities like CT, PET, and SPECT have undergone a significant transformation, offering enhanced methods for early and precise cancer diagnosis, therapy, and therapy response assessment. Concurrently, GATE has played a crucial role since its initial release in 2004, contributing to advancements in nuclear imaging, particularly in PET and SPECT imaging [8, 9]. GATE is extensively employed to characterize and optimize the image quality of scanners from major manufacturers (e.g., Siemens [10], General Electric [11], Philips [12]). It plays an important role in designing, optimizing, and validating new systems, addressing key parameters such as the detection medium, light collection system, and scanner geometry. GATE's contributions extend to prototype detector developments, shaping the next generation of imaging systems with innovations like heterostructured scintillators for ultra-fast TOF-PET scanners [13], total body acquisition [9], and Compton Camera systems [14]. Furthermore, GATE finds application in data correction and tomographic reconstruction, where the production of simulated data is pivotal for validating new algorithms aimed at improving quantitative analysis.

A recent topical review [15] delves into the latest developments in GATE Monte Carlo simulations, specifically tailored for emission tomography.

Optical imaging

GATE can be used for simulating optical imaging systems with bioluminescence[16], fluorescence [17], and Cerenkov luminescence [18]. The optical properties of biological tissues such as refractive index, absorption and scattering coefficients can be defined as a function of wavelength thereby allowing realistic simulations of optical imaging. Additionally, it supports Cerenkov luminescence simulations (see examples in Figure 4), serving as a key research tool in both nuclear medicine [19] and radiotherapy [20].

Positronium imaging

The GATE platform can be used as a tool to develop novel PET imaging methods beyond the conventional two-photons tomography. In particular, it is capable of simulating *positronium* decay, a bound atomic state of an electron and a positron, that is formed before annihilation occurs. The measurement of positronium properties, e.g. its mean lifetime, can provide supplementary information about the metabolic processes in the patient's body [21]. Positronium

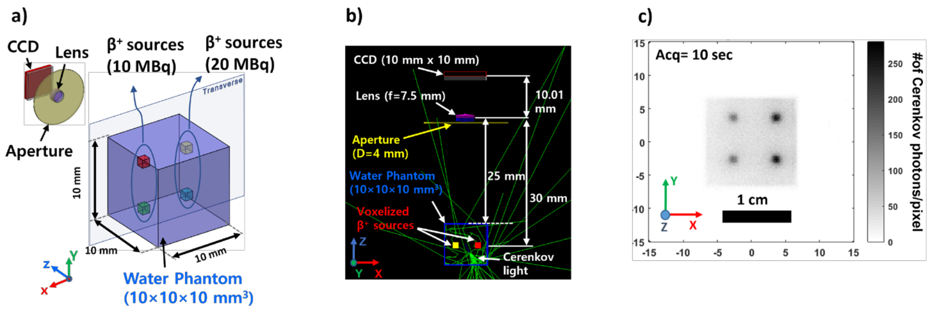

Figure 4. a) GATE Cerenkov luminescence imaging setup with optical imaging system and positron sources inside a water phantom, b) GATE Cerenkov luminescence imaging simulation geometry, c) the CCD image that collected Cerenkov luminescence light for 10 seconds.

imaging performance studies for several large-field-of-view plastic-based scanner prototypes have been described in [22].

X-ray imaging

GATE is extensively used in X-ray medical applications such as CT, dual-energy CT, Cone-Beam CT (CBCT), and mammography (example references can be found in [3]). The simulations contribute to both image enhancement methods, like scatter estimation, and patient dose calculations, including organ dose assessments. GATE also incorporates variance reduction techniques like Fixed-Forced Detection [23].

2.3 Dosimetry applications

External beam radiation therapy

GATE plays a crucial role in addressing complex challenges in photon radiotherapy, offering solutions for issues like dose calculations with large heterogeneities [24], skin dose for breast cancer treatments [25], and double calculations of radiotherapy treatment plans [26]. While less common for external photon beam therapy compared to other software, GATE has a significant impact in light ion beam therapy centers[27], especially with the Gate-RTion release. This project aims to simplify the integration of GATE in clinical centers. It offers a stable GATE release with validation tests for dosimetric applications in light ion beam therapy, providing essential tools for clinical users to interface GATE with the clinical environment. Moreover,a Gate-RTion-based independent dose calculation system for light ions (proton and carbon), IDEAL (Independent DosE cAlculation for Light ion beam therapy), is developed [28](available on the Git repository of OpenGATE).

Radionuclide therapy

Since the incorporation of radiation therapy and dosimetry applications in 2014 [29], GATE's impact on cancer research has increased, making it a gold standard for dosimetry calculations. The platform utilizes GEANT4 to emulate energy deposition in biological media, enabling dosimetry through Monte Carlo simulations, dose point kernels, and recent applications of deep learning for fast dose computation[30]. GATE has been used for image-based dosimetry

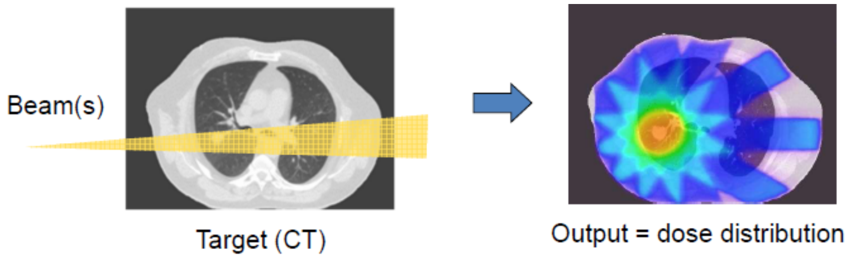

Figure 5. Illustration of GATE simulated dose distribution after radiotherapy treatment on a phantom.

in research and clinical practice [25, 31]. The platform combining high precision dosimetry and well-validated image modeling has the potential to become a tool of choice for investigating and developing approaches for use of new radionuclides for imaging and treatment.

Radiobiology

GATE is increasingly utilized to predict radiation effects at micro and nano scales, spanning preclinical cell irradiations to advanced hadrontherapy treatments [32]. It is the preferred tool for simulating preclinical or clinical beam characteristics detailed in a phase-space file, combined with GEANT4-DNA simulations [33] to assess radiobiological effects. To date, GATE is not able to fully handle multi-scale simulations from the calculation of dose to organs to an accurate identification and understanding of cellular and molecular damage. However, some separately working tools are available already such as C++ Cell POPulation modeler [34] integrating various cell population models. Upcoming developments will favor the integration of relevant features that have been tested so far through GEANT4-DNA simulations. Recently, specific actors are being developed for proton and carbon ion therapy to calculate LET or biological dose-based clinical treatment planning. In addition, the estimation of the biological dose will be proposed through the BioDoseActor [35].

3 Toward GATE v.10

GEANT4's existing `messenger` system, reliant on macro commands in text files, although powerful, exhibits limitations in user-friendliness, particularly when dealing with intricate simulation structures involving loops, variables, or computations. Recognizing Python's quality in data analysis, GATE collaboration explores the direct description of simulations in Python instead of traditional macro files. This novel approach planned to be released as GATE v.10 offers benefits such as the use of regular Python scripts also easily including artificial intelligence methods. The prototype code, leveraging the GEANT4 python binding through `pybind11`, demonstrates the feasibility of this methodology. The new GATE engine is bifurcated into Python, managing simulation initialization, and C++, handling tasks during runtime. While potential drawbacks include dual-language coding, the clear separation of initialization and runtime tasks into Python aims to simplify maintenance and development.

Beta version of GATE 10, already accessible on GitHub, is easily installed using the 'pip' package manager with a single command, supporting Linux, MacOS, and partially Windows. The user is relieved from manual GEANT4 installation as it comes pre-compiled with GATE 10. A robust development strategy mandates a test case for each GATE 10 feature, conducting over 140 automated simulations per code modification. These tests also serve as user examples.

The first experimental release, potentially evolving into the future GATE 10.x series, is anticipated in 2024.

4 Conclusion

The GATE Monte Carlo toolkit, a GEANT4-based platform for medical imaging and radiotherapy simulations, plays an important role in advancing the fields. Utilizing the GEANT4 engine, GATE simplifies complex simulations through a user-friendly macro language, aligning with the evolving GEANT4 toolkit with annual releases. GATE finds applications in both imaging and dosimetry domains, contributing to the design and optimization of imaging systems and radiation therapies. As an open-source, C++-based platform, GATE stands as a versatile and widely adopted tool, with ongoing developments expected to further enhance its capabilities and impact in the future.

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