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GATE 10: Towards a versatile python-driven Geant4 application for medical physics

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Background: GATE [1,2] is a long-standing Geant4 application dedicated to medical physics, e.g. nuclear imaging and radiation therapy systems. Since the beginning of GATE almost 20 years ago, users configure a simulation via Geant4-style macro commands grouped in text files. Since then, the rise of machine learning and high-level programming languages such as Python has revolutionized scientific computing. We present here the status of the future GATE 10 version featuring a Python-based scripting interface and integration of artificial intelligence methods.

Material and Methods: GATE 10 is composed of two core parts: first, a C++ library that exposes Geant4 as well as additional Gate-specific functions and classes via pybind11 [5]; second, a pure Python package providing a user interface to build simulations. This interface is designed to be as simple as possible for the user while offering a flexible infrastructure based on which developers can contribute additional functionality. The user has access to computational instruments commonly available in Python such as loops, conditionals, as well as external libraries for pre- and post-processing of data.

Simulations are divided into four main components: geometry (volumes, materials), physics (physics lists, cuts and other options), sources (definition of initial events) and actors (hooks into Geant4 actions, e.g. dose scoring, phase space recording, digitizer chains).

The user adds and configures these components via a Python syntax, which, behind the scenes, checks and ensures consistency of the user input. The configuration of a simulation is handled by a set of manager classes, which also provide various utility functions to inspect the simulation set-up.

The actual simulation run in Geant4 is performed by a set of engine classes which interact with the Geant4 library via bindings (pybind11). They also ensure correct memory and pointer management between Python and C++. The engines rely on the Geant4 RunManager, just like most conventional Geant4 applications. At the end of a run, the output is sent back to the Python-side of GATE 10 where the user can directly use it for further processing.

Like in previous GATE versions, voxelized images (e.g. based on CT images) and voxelized sources (e.g. based on emission tomography images) can easily be inserted from various image file formats. As a new feature in GATE 10, native Geant4 multithreading (MT) capability is available (for most features so far) – the user simply sets the number of threads. All Geant4-DNA chemistry constructors are included. Additionally, GATE 10 provides a mechanism to encapsulate the Geant4 simulation in its own subprocess. This allows GATE 10 to run multiple subsequent simulations in interactive Python environments such as ipython, jupyter notebook, or others. We plan to extend this mechanism in the future to provide automatic multiprocessing.

Preliminary results: GATE 10 is open-source and available via GitHub [4]. Installation is performed via the python package manager ('pip'), which allows for a simple installation process with one single command. All major platforms, i.e. Linux, MacOS, and Windows are supported, although the Windows version does not include all the features yet. The user is not required to manually install Geant4 as it ships pre-compiled with GATE 10.

The current version is 10.0beta06 which so far contains most of the features of the previous GATE 9. MT compatibility ensures an efficient use of computational resources and reduces post-processing efforts for the users. Part of our development strategy is that every feature in GATE 10 must have a test case to ensure code integrity over time. Currently, more than 140 test simulations are run automatically each time the code is modified. These tests also serve as examples for users. Several examples demonstrate the integration of artificial intelligence methods such as phase space generation via generative neural networks [3]. GATE 10 can be easily used by other software as an external library. For example, it is currently being integrated into the IDEAL 1.2 platform for independent dose calculation in light ion beam therapy [6] A first non-beta release is planned for May 2024.

[1] Jan S et al. GATE V6: a major enhancement of the GATE simulation platform enabling modelling of CT and radiotherapy. [Phys Med Biol. 2011](#)

[2] Sarrut D et al. The OpenGATE ecosystem for Monte Carlo simulation in medical physics. [Phys Med Biol. 2022](#)

[3] Saporta A et al. Modeling families of particle distributions with conditional GAN for Monte Carlo SPECT simulations. [Phys Med Biol. 2022](#)

[4] <https://github.com/OpenGATE/opengate>

[5] <https://github.com/pybind/pybind11>

[6] Grevillot, L., et al. The GATE-RTion/IDEAL independent dose calculation system for light ion beam therapy. [Front Phys 9. 2021](#)