

# Calzone: A Geant4 Python wrapper for the simulation of outdoor particle detectors

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## Software

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## Summary

The transport of high-energy particles (e.g., gamma-rays) through ordinary matter is an inherently stochastic process, with individual collisions described within the framework of quantum field theory. The resolution of such transport problems is facilitated by the use of Monte Carlo methods, denoted Monte Carlo particles transport (MCPT) herein. In particular, the [Geant4](#) software (Agostinelli et al., 2003; Allison et al., 2006, 2016) is an established MCPT C++ library for simulating the passage of high-energy particles through matter.

[Calzone](#) (CALorimeter ZONE) is a MCPT [Python](#) package built on top of [Geant4](#). It was developed in the context of geosciences with the objective of studying the emission of radioactivity from volcanoes (Terray et al., 2020), and in particular to simulate the response of gamma spectrometers deployed in the field. To this end, [Calzone](#) was developed in conjunction with [Goupi](#) (Niess et al., 2024), a backward gamma transport engine, and is interoperable with the latter. Yet, both packages can be used entirely independently, if necessary.

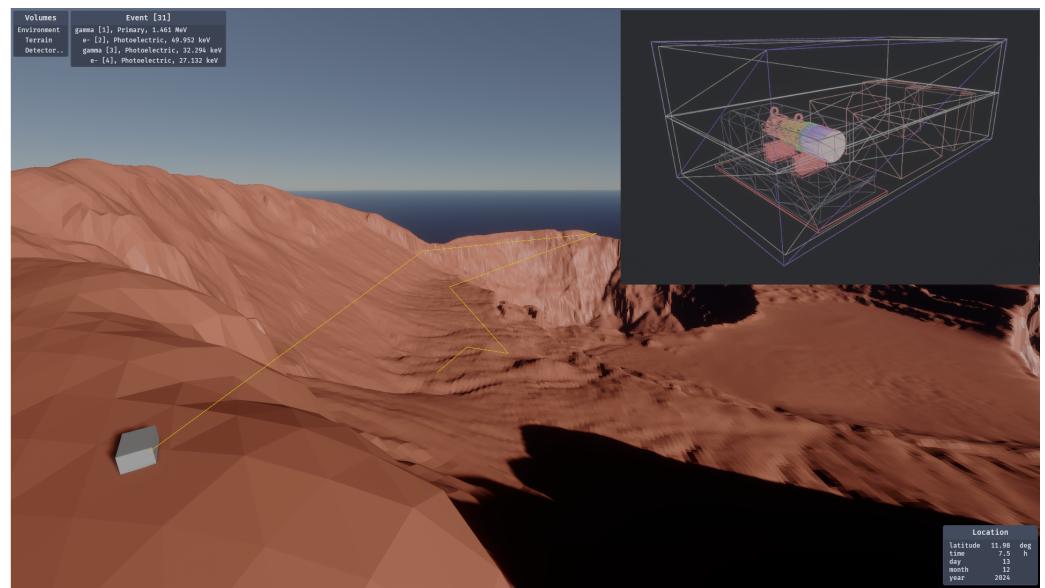
[Calzone](#)'s interface has been designed with simplicity in mind. Source particles are injected into the simulation volume as a [NumPy array](#) (Harris et al., 2020), and a [NumPy array](#) of collected energy deposits (or particles) is returned. The Monte Carlo geometry is encoded in a [Python](#) dict, which can be loaded from configuration files, e.g., using [JSON](#), [TOML](#) or [YAML](#) formats. This basic workflow is illustrated below,

```
simulation = calzone.Simulation("geometry.toml")
particles = calzone.particles(
    10000,
    pid="gamma",
    energy=0.5,      # MeV
    position=(0,0,1) # cm
)
deposits = simulation.run(particles).deposits
```

[Calzone](#) encourages the use of meshes to describe the Monte Carlo geometry. Various mesh formats are supported, such as OBJ, STL, GeoTIFF and [Turtle](#)/PNG (Niess et al., 2020). These formats can be used to encode the components of a detector (exported from a computer-aided design, or CAD, scheme) or a digital elevation model (DEM) describing the surrounding terrain. Additionally, [Calzone](#) features an interactive display ([calzone-display](#)) that allows users to navigate through the Monte Carlo geometry and to inspect Monte Carlo tracks (see, e.g., Figure 1).

## Statement of need

The [Geant4](#) software was designed as a generic toolkit, with the capability of being extended using the C++ inheritance mechanism. The software is provided under an open-source [licence](#) and is subjected to rigorous [validation](#) including comparisons with experimental data ([Allison et al., 2016](#)). As a result, [Geant4](#) is employed in a multitude of [applications](#), including high-energy physics (its initial scope) and radiation studies (e.g., for medical or space sciences).



**Figure 1:** Example of [calzone-display](#). The background image comprises a digital elevation model (DEM) of the Masaya volcano, derived from photogrammetry measurements. The grey box on the volcano ridge (bottom-left) corresponds to a gamma-spectrometer (located at 11.983056°N, 86.172815°W), the details of which are displayed in the top-right insert (using wireframe mode). The superimposed yellow segments illustrate the trajectory of a photon, originating from the 1.46 MeV emission line of  $^{40}\text{K}$ , simulated with [Calzone](#) and [Goupi](#) in conjunction.

However, the generic nature of [Geant4](#) implies a relatively low-level C++ [user interface](#). Thus, a number of software solutions have been developed on top of [Geant4](#), providing a higher-level user interface and extending its functionalities. This is exemplified by, but not limited to, [Gamos](#) ([Arce et al., 2014](#)), [Gate](#) ([Jan et al., 2004; Sarrut et al., 2022](#)), [Geant4Py](#), [Gras](#) ([Santin et al., 2005](#)) and [Topas](#) ([Faddegon et al., 2020; Perl et al., 2012](#)).

In the context of geosciences, we encountered specific issues that were not addressed by [Geant4](#), and only partially addressed by some of its derivatives. Some of these issues, which motivated the development of [Calzone](#), are discussed hereafter.

## Selected Calzone features

This section outlines a number of key features of the [Calzone](#) package, along with the specific issues that these features address.

### Native mesh support

The precision of MCPT computations is contingent upon the accuracy of the geometry description. In the context of geosciences, the aforementioned geometry includes the particle detector, which is depicted in a mechanical diagram (using a CAD software), as well as the

study site, which is usually represented by a digital elevation model (DEM). These data are not natively understood by `Geant4`, requiring transcription. A generic approach is to delineate volumes of the same material (terrain, sensor, mechanical support, etc.) using surfaces approximated by triangular meshes. For instance, the `FreeCAD` software is able to export the detector parts as STL files, which could then be re-read and transcribed into `G4TessellatedSolids` (e.g., using `CADMesh`) (Poole et al., 2012). `Calzone` streamlines this process by defining a geometry format that serves as an intermediary. This format uses standard objects, including dict, float, list, and str, and integrates various mesh formats, such as OBJ, STL, GeoTIFF and `Turtle`/PNG (Niess et al., 2020). `Calzone` then translates this data into `Geant4` objects.

## Mesh specialisation

The process of meshing a DEM with triangular facets introduces specific issues. To optimise the geometry traversal, the `Geant4` software uses a voxelisation algorithm. This method scales poorly for DEMs that typically comprises millions of nodes (Niess et al., 2020), and is inefficient for long-range particles (such as  $\gamma$  and  $\mu$ ). Thus, `Calzone` defines a dedicated Mesh object that includes a bounding volume hierarchy (BVH) algorithm (partitioning the surface of the mesh, rather than its volume). The user may then select the desired algorithm for each mesh. The default approach is to use a surface BVH for DEMs, while voxelisation is used otherwise (i.e., a `G4TessellatedSolid`).

## Interoperability with `Goupi`

A further distinctive feature of MCPT applications in geosciences (such as gamma-spectrometry and muography) is that the source largely encompasses the detector, which renders analogue simulations ineffective. In a typical use case, only a few dozen out of a million of simulated particles leave a signal in the detector. It is therefore often necessary to rely on importance sampling methods. One effective method in this context is to backward simulate the transport in the detector's far environment (Niess et al., 2018; Niess, 2022). To this end, `Calzone` is interoperable with `Goupi` (Niess et al., 2024).

## Particles generator

Another point of interest for MCPT applications is the modelling of particle sources. For this purpose, `Calzone` provides a geometry-aware `ParticlesGenerator` object, which can, for instance, generate particles entering a specific geometry volume. Moreover, `Calzone`'s `ParticlesGenerator` consistently provides generation weights, which are essential for importance sampling methods.

## Software architecture

The `Calzone` application was developed in `Rust`, with a `Python 3` user interface (using the `PyO3` crate). Interfacing with `Geant4` was facilitated by the `Cxx` crate. The interactive visualisation was implemented using the `Bevy` game engine.

## Author contributions

An initial C++ prototype of `Calzone` was developed by K.V. and V.N. Subsequently, V.N. ported `Calzone` to `Rust` and extended its functionalities. L.T. was instrumental in initiating, advising and supervising this project. All authors contributed to the preparation of this manuscript.

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