PYG4OMETRY: a Python library for the creation of Monte Carlo radiation transport physical geometries

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Abstract
Creating and maintaining computer-readable geometries for use in Monte Carlo Radiation Transport (MCRT) simulations is an error-prone and time-consuming task. Simulating a system often requires geometry from different sources and modelling environments, including a range of MCRT codes and computer-aided design (CAD) tools. PYG4OMETRY is a Python library that enables users to rapidly create, manipulate, display, debug, read, and write Geometry Description Markup Language (GDML)-based geometry used in MCRT simulations. PYG4OMETRY provides importation of CAD files to GDML tessellated solids, conversion of GDML geometry to FLUKA and conversely from FLUKA to GDML. The implementation of PYG4OMETRY is explained in detail in this paper and includes a number of small examples to demonstrate some of its capabilities. The paper concludes with a complete example using most of PYG4OMETRY’s features and a discussion of possible extensions and future work.

Keywords: Geant4; FLUKA; GDML; CAD; STEP; Monte Carlo; Particle; Transport; Geometry;

PROGRAM SUMMARY
Program Title: PYG4OMETRY
Licensing provisions: GPLv3
Programming language: Python, C++
External routines/libraries: ANTLR, CGAL, FreeCAD, NumPy, OpenCascade, SymPy, VTK

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Nature of problem:
Creating computer-readable geometry descriptions for Monte Carlo radiation transport (MCRT) codes is a time-consuming and error-prone task. Typically these geometries are written by the user directly in the file format used by the MCRT code. There are also multiple MCRT codes available and geometry conversion is difficult or impossible to convert between these simulation tools.

Solution method:
Create a Python application programming interface for the description and manipulation of Geant4 and FLUKA geometries, with full support for the direct reading and writing of their respective geometry description file formats. Form triangular meshes to represent geometric objects for both visualisation of the geometry and to enable the use of advanced mesh-based geometric algorithms. Triangular mesh processing algorithms allow the loading and use of STL and CAD/CAM files. Converting from FLUKA to Geant4 requires algorithms to decompose solids to a set of unions of convex solids. Converting from FLUKA to Geant4 requires a number of steps including the replacement of infinite surfaces with finite solids and the automatic elimination of overlaps.

1. Introduction

There are numerous different software codes to simulate the passage of particles through material, such radiation transport (RT) programs include MCNP [1], FLUKA [2, 3], Geant3 [4] and Geant4 [5]. All these codes are based on the Monte Carlo technique but each code either has a particular specialism, simulation methodology or target user community. Monte Carlo RT (MCRT) simulations have diverse uses including shielding calculations for radiological protection, detector performance, medical imaging and therapy, and space radiation environment simulations. A fundamental requirement of all of the codes is to supply a computer-readable description of the physical 3D geometry that the particles are passing through. The creation of geometry files is typically a very time-consuming activity and the simulation validity and performance is directly dependent on the quality of the geometry. There is no standard geometry format used across MCRT codes, with each code often using its own unique format. A user will typically not have geometry in both FLUKA and Geant4 for example. A geometry system that enables the conversion between files prepared for different codes will allow for cross-checks of the physics processes in different particle transport codes. The file formats used for geometry are generally focused on the computational efficiency of particle tracking algorithms and not ease of preparation. In
addition to the creation of geometry files for RT programs, usually computer-aided design (CAD) files exist for systems which need to be simulated. The fundamental geometric representations in CAD files are usually not amenable to MCRT programs. For these reasons it is advantageous to create a software tool that allows particle transport code users to rapidly develop error-free geometry files, convert between common MCRT geometry formats and load CAD models.

This paper describes a geometry creation and conversion package called PyG4ometry, written in Python and internally based on the Geant4 application programming interface (API) and the Geometry Description Markup Language (GDML) for file persistency [6]. The main features of PyG4ometry are a Python scripting API to rapidly design parametrised geometry; conversion to and from FLUKA geometry descriptions; conversion from CAD formats (STEP and IGES) based on FreeCAD [7] and OpenCascade [8]; and powerful geometry visualisation tools based on VTK [9]. The origin of PyG4ometry was a set of utilities to prepare geometry for an accelerator beamline simulation program based on Geant4 called BDSIM [10]. Accelerator physicists, like specialists in other areas, need a tool to quickly model specialist geometry and the subsequent interaction of the charged particle beam. PyG4ometry allows the rapid creation and adaptation of geometry, with Figure 1 demonstrating various possible workflows. PyG4ometry is not an executable software package but a toolkit, a user would typically write a very small Python program to use the classes and functions provided by PyG4ometry. This paper describes version 1.0 of PyG4ometry, which is freely available as a Git repository and via the Python Package Index (PyPi).

![Figure 1: Schematic of PyG4ometry workflow, showing (a) the different input file formats, (b) Python processing, (c) output file targets and (d) MCRT codes which use the geometry.](image-url)
There are existing codes that have functionality similar to Pyg4ometry. ROOT [11], the high-energy physics data analysis framework, can load, display and manipulate GDML-like geometry. Existing open source tools to convert CAD files to GDML include GUIMesh [12], with commercial solutions including ESABASE2 [13] and FASTRAD [14]. There are also tools from the fusion and neutronics community that can convert CAD geometry into formats usable by MCRT codes, with examples including DAGMC [15] and MCCAD [16]. In principle CAD software can export shape data to STL (or other similar mesh formats), which can be used by Geant4 [17]. However, in practice using a lot of CAD models is difficult if that model is composed of a large number of parts. This is because exporting, assigning material to, and placing the STL components into the MCRT code can be very cumbersome. Almost all modern CAD tools such as CATIA, Inventor and SolidWorks have a scripting language to allow users to programmatically generate geometry. Similar CAD-style scripting languages do not exist for either GDML or FLUKA and the existent set of software does not provide a complete set of tools to efficiently create complex geometries for these codes.

This paper is structured as follows, first a brief radiation transport-focused introduction to computer descriptions of geometry and an explanation of the design and implementation of Pyg4ometry. Subsequent sections describe how Pyg4ometry can be used to perform rapid geometric modelling as well as conversions from FLUKA to GDML, GDML to FLUKA and CAD to GDML. The paper concludes with an example of a composite, complex system consisting of components drawn from all the supported geometry input file formats.

2. Computer descriptions of geometry

Central to a computer-readable geometry is how a solid is defined in three dimensions. There are numerous different ways to describe a geometry, including constructive solid geometry (CSG), boundary representation (BREP) and tessellated polygons, which are described briefly in this section. The Geant4 geometry specification is a mixture of all three of these geometry modelling techniques and described in detail last.

Constructive solid geometry uses Boolean operations (subtraction, intersection and union) between simple solid shapes (e.g. cube, cylinder, sphere, etc.) or infinite volumes (e.g. a plane-defined infinite half-space) to model complex surfaces which represent a solid. Boolean operations and solids
can be combined to form a CSG tree to model complex geometry. FLUKA uses CSG to model solids, however the form of Boolean expression used by FLUKA is not a general CSG tree but a logical expression in disjunctive normal form.

Boundary representation consists of two parts, topology and geometry. Topological elements are faces, edges and vertices and the corresponding geometrical elements are surfaces, curves and points. No current MCRT applications use native file formats employed by CAD systems. The conversion of CAD BREP formats for loading in MCRT applications is typically performed via a tessellated format, although it is possible to decompose BREP descriptions to bounded or infinite mathematical surfaces and subsequently solids as used in CSG descriptions. This type of conversion is complex and error-prone, although recent progress has been made [18].

Solid volumes can be defined using triangular, quadrilateral or tetrahedral meshes. Numerous formats exist to describe meshes, the ubiquitous being STL with more modern examples including PLY and OBJ. For solids with curved faces a tessellated mesh will always give an approximate description. As the mesh deviation distance from the solid decreases the number of polygons increases and with it the memory consumption and execution time of the MCRT simulation.

Geant4 geometry description is the richest and most flexible of MCRT codes and consists of a mixture of BREP, CSG and tessellated concepts. Geant4 includes 27 basic solids and it does not store a sense of topology present in traditional CAD BREP systems. One of the fundamental solids is a tessellated solid which can be used to represent STL or PLY files. Geant4 also provides the ability to perform Boolean operations on these primitive solids. Not only do solid objects need to be defined but also placed in a world coordinate system. Geant4 has two concepts which facilitate this: logical volumes and physical volumes. A logical volume is a region of space that is defined by an outer solid but also other attributes like material, magnetic field and zero or more daughter physical volumes. A physical volume is a unique placement (or instance) of a logical volume. This design permits large reuse of objects, minimising memory footprint for largely repetitive structures such as detectors that Geant4 was created to simulate.

If a user is creating and placing multiple daughter volumes within a mother volume then it is the user’s responsibility to create a solid which fully encompasses the daughter volumes. Overlaps between daughter volumes and the mother can be detected, but it is desirable to have a mother
volume shape that efficiently holds its daughters. However, there are exceptions to this rule in the form of assembly volumes.

To exchange geometry descriptions between software packages the Geometry Description Markup Language (GDML) was developed [6]. GDML is an XML-based description of Geant4 geometry. Geant4 and ROOT [19] can read and write GDML and it is commonly used as an exchange format for Geant4 geometries.

3. PYG4OMETRY design and layout

PYG4OMETRY is a Python package consisting of semi-independent sub-packages. The sub-package pyg4ometry.geant4 contains all classes for Geant4 detector construction and pyg4ometry.gdml provides the functionality for reading and writing GDML files. There are sub-packages for importing and exporting other geometry formats: pyg4ometry.fluka, pyg4ometry.stl and pyg4ometry.freecad. Lastly, the sub-package pyg4ometry.convert is used for conversions between formats.

The core of PYG4OMETRY consists of Python classes that mimic Geant4 solids, logical volumes, physical volumes, GDML parameters and material classes. The constructors of the Python classes are kept as close to the original Geant4 C++ implementation as possible so that PYG4OMETRY users do not have to learn a new API. For example the G4Box class in Geant4, has the XML tag box in GDML and is represented by the Box class in PYG4OMETRY. The Python object initialisers are very similar to their corresponding Geant4 C++ constructors, but the length definitions are those used by GDML. For example, GDML uses full-lengths whilst Geant4 uses half-lengths. Geometry construction in Python proceeds in a way which is very similar to geometry construction in Geant4. A user relatively familiar with Geant4 should be able to start creating geometry in PYG4OMETRY immediately. In the rest of this section novel or important developments in PYG4OMETRY are described.

For each input format supported by PYG4OMETRY (GDML, STL, FLUKA and STEP) a dedicated Reader class is implemented: gdml.Reader, stl.Reader, fluka.Reader and freecad.Reader. Each reader constructs the appropriate PYG4OMETRY classes and provides a Registry instance which can be used or manipulated by the user. Output consists of taking the registry and writing to file with the desired format.

The internal data representation closely follows the structure of GDML. A Registry class aggregates Python ordered dictionaries that are used to store
the main elements of a GDML file. As a PyG4ometry user instantiates the
gamey the associated registry (typically provided as a keyword argument
to the class initialiser) is updated. When a user is finished with the geometry,
the registry can be written to disk as a GDML file. It is also possible to
modify Registry instances, for example by adding or removing volumes, or
by combining with other instances to form an aggregate.

In GDML symbolic expressions can be used to parametrise solids and
their placements. These expressions are evaluated when the GDML is loaded
into Geant4. In order to fully replicate the functionality of GDML an ex-
pression engine was implemented using ANTLR [20]. The GDML is loaded
using standard XML modules and parsed using ANTLR to create an ab-
stract syntax tree (AST). GDML allows for the definition and assignment of
variables. GDML expressions are not much more complicated than binary
operators $+,-,\times,/$ and common trigonometric and special functions. The
AST terminates on either expressions which evaluate to numbers or GDML
variables. Internally, all PyG4ometry classes use GDML expressions and
not floating-point numbers. Storing internal data as expressions allows for de-
ferred evaluation (or re-evaluation) of solid parameters and placements. This
allows a user to update variables whilst defining geometry and the expression
engine will update all internal values. An example of GDML expressions is
shown in Listing 1.

Listing 1: A simple Python script using PyG4ometry to create GDML variables.

```python
# Import modules
import pyg4ometry

# Create empty data storage structure
reg = pyg4ometry.geant4.Registry()

# Expressions
v1 = pyg4ometry.gdml.Constant("v1","0",reg)
v2 = pyg4ometry.gdml.Constant("v2","sin(v1+pi)",reg)
```

A powerful feature of Geant4 and hence GDML is the ability to either
repeat, divide or parametrise geometry. The class which enables the creation
of multiple replicas of a volume in a Cartesian, cylindrical or spherical grid
is known as a Replica Volume. A Division Volume breaks a primitive into
segments in either Cartesian or cylindrical polar coordinates. A parametrised
volume allows for the arbitrary multiple placement of solids where the pa-
Parameters are allowed to vary for each placement. Another way in GDML to create parametrised solids or volumes is GDML loops, where sections of GDML can be repeated with varying parameters based on the loop index. GDML loop loading and expansion are not supported by PyG4ometry but will be implemented in a future release.

3.1. Tessellation of solids (meshing)

Creating a uniform 3D mesh description of all solids (including Booleans) is exceptionally useful for visualisation and other algorithms, such as overlap detection. For each Geant4 solid instance a triangular tessellated vertex-face mesh is generated and cached. This mesh is then used to determine the extent of placed instances of geometry (physical volumes) and meshes for CSG-derived solids. CSG mesh calculations are performed using a Binary Space Partitioning (BSP) tree technique in pure Python [21] or via the Computational Geometry Algorithms Library (CGAL) surface meshes [22] in C++. The pure Python CSG backend is further accelerated by compiling it to C using Cython [23]. For maximum flexibility either backend can be used, but in general the CGAL implementation is one to two orders of magnitude faster than the Cythonized CSG implementation and should be preferred, particularly for large geometries. Triangular meshes based on CSG operations involving curved surfaces often contain large numbers of triangles. Before meshes are visualised or written to file various polygon mesh algorithms from CGAL [24] can be employed to give the meshes more desirable features.

3.2. Visualisation

When implementing geometry a rapid and robust visualisation system is key to produce error-free and efficient simulation input. A PyG4ometry geometry hierarchy can be viewed using the popular Visualisation Toolkit (VTK). No separate scene graph is required as the Geant4 volume hierarchy is sufficient to place the meshes associated with each physical volume. A daughter volume is placed within a logical volume with a rotation $R_d$, reflection $S_d$ and translation $T_d$.

The transformation $M$ and translation $T$ from mother to daughter is

$$M = S_d R_d,$$  \hspace{1cm} (1)  $$T = T_d.$$  \hspace{1cm} (2)
If the mother volume is placed in the world then the placement transformation $M_w$ and translation $T_w$ are expressed as

$$M_w = M_m M_d = S_m R_m S_d R_d,$$

$$T_w = M_m T_d + T_m = S_m R_m T_d + T_m,$$

where the subscript $m$ indicates mother volume and $d$ indicates daughter volume. Given a hierarchy of logical and physical volumes, Equations 3 and 4 can be used recursively to place an arbitrary number of nested volumes.

The physical volume class ($\text{geant4.PhysicalVolume}$) is also used to store visualisation attributes like the solid’s colour, surface or wire-frame representation and visibility. Overlaps detected in the mesh geometry are stored in the $\text{LogicalVolume}$ instance and can be displayed separately to allow a user to visually identify and debug the overlaps.

Geometry needs to be augmented with other information for a complete MCRT simulation. Often, other attributes need to be assigned to regions of space, for example material definition, magnetic field or optical properties. These physical properties can be used to define the visualisation attributes of a volume.

### 3.3. Overlap detection

All MCRT codes cannot handle spatial overlap between two geometric objects and will have ill-defined behaviour when tracking particles in such a situation. A key feature of PYG4OMETRY is the detection of potential overlaps in a way which is most useful to the user, it does this by performing an
intersection operation between solid instances and determining if the resulting mesh is empty. Figure 3 shows three different types of possible overlaps, (a) protrusion of a daughter from the mother, (b) finite volume intersection between two daughters and (c) an overlap where two daughters share a face. If the resulting intersection is non-null then the overlaps can be displayed side-by-side in the visualisation.

![Figure 3: schematic of the three different types of overlap between the daughters of a mother logical volume.](image)

Overlap detection in **PyG4ometry** relies on the meshes generated for each solid. As these mesh representations will generally approximate their respective solid, so to will any overlap detection algorithm be an approximation. Generally, the overlap detection algorithm proceeds as shown in Algorithm 1. For a logical volume with \( n_{\text{daughters}} \) physical volumes, assuming meshes for solids have an average number of faces \( n \), clearly this algorithm has complexity \( \mathcal{O}(n^2 n_{\text{daughters}}^2) \). This complexity can result in a steep computational cost for highly-flat geometry hierarchies, but overall remains worthwhile considering the potential waste in large amounts of cluster CPU time if small overlaps are present in the final MCRT simulation. This algorithm clearly favours geometry descriptions which have a high degree of logical volume reuse, however this is also true of Geant4 as a whole, so the user will likely be inclined to design along such lines regardless. Due to the discrete nature of triangular meshes it is not possible to have perfect detection of overlaps, especially when curved surfaces are considered, and in some rare cases either overlaps maybe missed, or spurious overlaps maybe reported. However, the density of the meshes created for the solids is controllabe by the user, meaning that the user can opt for more precise overlap detection.
Algorithm 1: The overlap checking algorithm employed in PyG4ometry. The algorithm proceeds by performing the CSG intersection of pairs of daughter volume meshes for a given logical volume. Non-null intersections between daughter volume meshes are treated as overlaps.

**Data:** Logical volume \( v \) with mesh \( m \) and daughter volume meshes \( d \in D \).

**Result:** Set \( S \) of non-null mesh intersections.

**Function** \( \text{Intersection}(n_1, n_2) \)

- **Data:** CSG meshes \( n_1 \) and \( n_2 \).
- **Result:** The mesh intersection of \( n_1 \) and \( n_2 \).

\[
V \leftarrow \emptyset; \\
S \leftarrow \emptyset; \\
\text{// Cache tried mesh pairs.}
\]

for \( d_1 \in D \) do

\[
p \leftarrow \text{Intersection}(m, d_1);
\]

if \( p \) is not null then

\[
S \leftarrow S \cup \{p\};
\]

for \( d_2 \in D \) do

\[
\text{if } d_1 = d_2 \text{ or } (d_2, d_1) \in V \text{ then}
\]

\[
\text{continue;}
\]

\[
q \leftarrow \text{Intersection}(a, b);
\]

if \( q \) is not null then

\[
S \leftarrow S \cup \{q\};
\]

\[
V \leftarrow V \cup \{(d_1, d_2)\};
\]

checking at the cost of greater computation time. In general, the overlap detection algorithm can present the potential overlaps quickly and easily to the user, thus significantly aiding the design process.

4. Rapid geometry modelling

Given the Python scripting interface, expression and tessellation engines it is possible for a user to rapidly specify the geometrical layout of the RT problem, vary the parameters of the geometry and visualise it. When a user has achieved the desired geometry without geometry overlaps, a GDML file
can be written from the internal memory representation. An example of some of the geometry scripting capabilities of PyG4ometry is shown in Listing 2. The structure should be familiar to regular users of Geant4 or GDML, apart from the new class described in the previous section called the Registry. First the Registry is created to store all the PyG4ometry objects; followed by constants; then materials, solids, logical volumes, physical volumes and other properties such as visualisation attributes; and finally the whole geometry can be saved as a GDML file or visualised using VTK.

Listing 2: A simple Python script using PyG4ometry to create a simple Geant4 geometry.

```python
# import modules
import pyg4ometry.gdml as gd
import pyg4ometry.geant4 as g4
import pyg4ometry.visualisation as vi

# create empty data storage structure
reg = g4.Registry()

# expressions
wx = gd.Constant("wx","100",reg)
wy = gd.Constant("wy","100",reg)
wz = gd.Constant("wz","100",reg)
bx = gd.Constant("bx","10",reg)
by = gd.Constant("by","10",reg)
bz = gd.Constant("bz","10",reg)
br = gd.Constant("br","0.25",reg)

# materials
wm = g4.MaterialPredefined("G4_Galactic")
bm = g4.MaterialPredefined("G4_Fe")

# solids
wb = g4.solid.Box("wb",wx,wy,wz,reg)
b = g4.solid.Box("b",bx,by,bz,reg)

# structure
wl = g4.LogicalVolume(wb, wm, "wl", reg)
bl = g4.LogicalVolume(b, bm, "b", reg)
```
bp1 = g4.PhysicalVolume([0,0,0],
                       [0,0,0],
                       bl, "b_pv1", wl, reg)
bp2 = g4.PhysicalVolume([0,0,-br],
                       [-2*bx,0,0],
                       bl, "b_pv2", wl, reg)
bp3 = g4.PhysicalVolume([0,0,2*br],
                       [2*bx,0,0],
                       bl, "b_pv3", wl, reg)

reg.setWorld(wl.name)  # define world volume

# physical volume visualization attributes
bp1.visOptions.color = (1,0,0)
bp1.visOptions.alpha = 1.0
bp2.visOptions.color = (0,1,0)
bp2.visOptions.alpha = 1.0
bp3.visOptions.color = (0,0,1)
bp3.visOptions.alpha = 1.0

# gdml output
w = gd.Writer()
w.addDetector(reg)
w.write("output.gdml")

# visualisation
v = vi.VtkViewer(size=(1024,1024))
v.addLogicalVolume(wl)
v.addAxes()
v.view()

An example of the VTK output for code Listing 2 is shown in Figure 4. Significantly more complex geometries can be developed using a structure similar to that shown.

The Pyg4ometry Python code in the example is approximately as expressive as the GDML it writes. The benefit of wrapping GDML in Python is that it allows very rapid prototyping of geometry without the overhead of C++ compilation (in the case of implementing the geometry directly in
Figure 4: VTK visualisation output from code Listing 2.
Geant4) or writing well-formed XML (in the case of GDML). Effectively, by using Pyg4ometry, the set of possible user-errors when describing geometry in C++ or XML instead either manifest as Python exceptions or are eliminated entirely. Another key benefit is the ability to use the Pyg4ometry code to create programmatic converters between different geometry languages or more generally manipulation and transformation of the geometry stored in memory. The rapid modelling example given in Listing 2 and Figure 4 is rather trivial, a significantly more complex example is shown in Figure 7.

5. FLUKA to GDML conversion

FLUKA geometry is based upon a limited set of primitives (referred to as bodies) which can be combined using Boolean operations. A zone consists of one or more bodies or subzones combined using intersections and subtractions. Zones may then be further combined using union operations to form regions, which are defined as the union of one or more zones, as well as a material.

Each FLUKA body is represented in Pyg4ometry with a corresponding class, and in turn each class has a method that returns a GDML primitive solid and a method that returns that solid’s rotation and position such that it matches its FLUKA equivalent. The expansion, translation and transform geometry directives are each folded into one or more of these three methods. The mapping of FLUKA bodies to GDML solids is shown in Table 1. It is worth noting that many of the FLUKA bodies are infinite in extent, but are mapped to finite GDML solids. The translation of infinite bodies to equivalent finite solids is one of the main and most involved steps in the conversion process. This mapping is possible because whilst FLUKA bodies can be infinite in extent, all zones and regions must be finite. Zones and regions are then composed by instantiating their respective classes and adding body instances to them. Each Zone and Region instance can then return its equivalent GDML Boolean solid.

The FLUKA CSG ASCII is parsed using an ANTLR4-generated parser, producing an AST. The resulting AST is then inspected sequentially (walked) to populate Region instances with zones and bodies. With the Region instances populated they can then be manipulated and translated into GDML. The translation involves a number of special steps to bridge the two disparate formats and ensure the resulting GDML is well-formed and usable in Geant4. Some of these steps are simple, for example in FLUKA unions can be dis-
Figure 5: Example conversion of a simple FLUKA geometry to GDML. Above: the original FLUKA geometry displayed in flair, FLUKA’s graphical user interface. Below: the GDML geometry viewed using PyG4ometry’s VTK visualiser. The example is a Faraday cup used to capture and measure accelerator beam charge.
connected, but in Geant4 specifically only multi-unions can be disconnected. Therefore, multi-unions are used throughout the converted geometry instead of the more conventional binary unions. Other procedures are more involved and are discussed in the rest of this section.

Listing 3: A simple PYG4METRY Python script to load a FLUKA file and convert its geometry to a Geant4 logical volume.

```python
import pyg4ometry.fluka as fluka
from pyg4ometry.convert import fluka2Geant4

reader = fluka.Reader("FlukaFileName.inp")
g4Registry = fluka2Geant4(reader.flukaregistry)
logical = g4Registry.getWorldVolume()
```

| FLUKA body                                      | PYG4METRY class       |
|------------------------------------------------|-----------------------|
| RPP (Rectangular parallelepiped)                | Box                   |
| BOX (General rectangular parallelepiped)        | Box                   |
| SPH (Sphere)                                    | Orb                   |
| RCC (Right circular cylinder)                   | Tubs                  |
| REC (Right elliptical cylinder)                 | EllipticalTube        |
| TRC (Truncated Right Angle Cone)                | Cons                  |
| ELL (Ellipsoid of Revolution)                   | Ellipsoid             |
| WED/RAW (Right Angle Wedge)                     | ExtrudedSolid         |
| ARB (Arbitrary Convex Polyhedron)               | TessellatedSolid      |
| XYP (X-Y Infinite half-space)                   | Box                   |
| XZP (X-Z Infinite half-space)                   | Box                   |
| YZP (Y-Z Infinite half-space)                   | Box                   |
| PLA (Generic infinite half-space)               | Box                   |
| XCC (X-axis Infinite Circular Cylinder)         | Tubs                  |
| YCC (Y-axis Infinite Circular Cylinder)         | Tubs                  |
| ZCC (Z-axis Infinite Circular Cylinder)         | Tubs                  |
| XEC (X-axis Infinite Elliptical Cylinder)       | EllipticalTube        |
| YEC (Y-axis Infinite Elliptical Cylinder)       | EllipticalTube        |
| ZEC (Z-axis Infinite Elliptical Cylinder)       | EllipticalTube        |
| QUA (Quadric surface)                           | TessellatedSolid      |
5.1. Infinite bodies

The majority of bodies in FLUKA are infinite in extent, and fall broadly into four categories, half-spaces, infinitely-long cylinders, infinitely-long elliptical cylinders and quadric surfaces. Translating these bodies to Geant4 requires generating the equivalent finite solid whilst retaining the same final finite Boolean shape. This is achieved with the use of axis-aligned bounding boxes (AABBs), in which the FLUKA body is translated to a finite solid with dimensions slightly larger than the AABB. The lengths of infinite (elliptical) cylinders are reduced to finite equivalents with lengths slightly greater than the bounding box. Similarly, half-spaces are reduced to boxes with one face acting as that of the half-space face, and quadric surfaces are sampled only over the volume denoted by the AABB. Furthermore, the positions of these solids are moved as close to the bounding box as possible whilst retaining an identical final Boolean geometry. Resizing and translating all bodies with respect to the region bounding boxes ensures that an identical region geometry can be generated, albeit from much smaller constituent bodies.

Generating these bounding boxes over which the bodies should be translated to GDML involves first evaluating each region with very large Tub, EllipticalTube and Box instances (by default 50 km in length), such that they are effectively infinite for most reasonable use cases. Py4ometry’s CSG meshing is then used to generate a mesh for each region from which the axis-aligned bounding box can be extracted. Each region is then evaluated a second time with respect to its bounding box, with all of its constituent infinite solids being reduced in size as described above. The implementation is described in Algorithm 2. This algorithm works robustly for half-spaces, infinite circular cylinders and infinite elliptical cylinders as the number of facets belonging to the mesh for such solids is independent of the size of the solid, so generating the initial mesh from arbitrarily large solids works well. Generating a quadric surface over a very large volume in space whilst retaining topological information is computationally very expensive, so to resolve this the user must provide the approximate axis-aligned bounding box of any region in which a quadric is used to constrain the size of the mesh only to where it is needed.

5.2. Removing redundant half-spaces

The above algorithm for replacing infinite FLUKA bodies with finite Geant4 solids works well in most cases, but additional care must be taken for redundant infinite half-spaces. A redundant infinite half-space is defined
Algorithm 2: The infinite-body minimisation algorithm employed in the conversion of FLUKA to GDML.

**Data:** FLUKA regions to be converted to GDML.

**Result:** GDML solids equivalent to the FLUKA regions built from minimally-sized primitive solids.

**Function** ToGDMLSolid(\(b, a\))

- **Data:** FLUKA body \(b\) with axis-aligned bounding box \(a\).
- **Result:** GDML solid equivalent to \(b\) bounded by the volume \(a\).

**Function** RegionAABB(\(r\))

- **Data:** FLUKA region \(r\).
- **Result:** Axis-aligned bounding box (AABB) of the FLUKA region.

\[
B \leftarrow \emptyset; \quad \text{// Map of regions to AABBs.}
\]

for \(r\) in regions to be converted do

\[
B[r] \leftarrow \text{RegionAABB}(r)
\]

// Map of bodies to minimal bounding boxes.

\[
E \leftarrow \emptyset;
\]

for \(b\) in bodies in regions to be converted do

for \(r\) in regions in which body \(b\) is used do

\[
E[b] \leftarrow E[b] \cup \text{RegionAABB}(r);
\]

\[
G \leftarrow \emptyset;
\]

for body \(b\) and AABB \(a\) in \(E\) do

// Map the FLUKA bodies to minimal GDML solids by converting with the minimal AABB, \(a\).

\[
G \leftarrow \text{ToGDMLSolid}(b, a);
\]

for \(r\) in regions to be converted do

build the corresponding GDML for \(r\) from the set of minimal GDML primitives in \(G\).
as one which has no effect on the shape of the final Boolean solid. Whilst this may be true of arbitrary bodies, it is most problematic for half-spaces. If the half-space is far away from the region’s AABB after the infinite body reduction has been performed, then it can result in a malformed Boolean. Such half-spaces are filtered from their respective regions during the conversion process by calculating the nearest distance from the centre of the AABB to the half-space face. If this distance is greater than the centre-to-corner distance of the AABB, then that half-space is deemed to be redundant with respect to that region and is removed from it during conversion.

5.3. Coplanar faces

Coplanar faces present a problem during conversion where the faces of two union components or that of two regions are perfectly coplanar in FLUKA. Coplanar faces of this nature are ubiquitous in FLUKA and present no problems to the operation of the program. However, in Geant4 these will generally result in tracking errors. These must be handled robustly to ensure the resulting geometry is usable in Geant4. Coplanar faces are resolved automatically by slightly decreasing the size of every body that is used in an intersection, and increasing the size of every body used in a subtraction. These rules are inverted for nested subtractions. This algorithm ensures that all coplanar faces are removed and replaced with resolvable, small gaps between faces. This approach works well for guaranteeing well-formed geometry that is free from tracking errors in Geant4.

5.4. Materials

Any useful translation between geometry description formats must also account for materials, and accordingly PyG4ometry correctly translates FLUKA materials to GDML. FLUKA materials can be divided into built-in, single-element and compound materials. Built-in materials are simply those that are predefined by FLUKA, single-element materials are described with a single MATERIAL card, and compound materials are described with one MATERIAL card followed by one or more COMPOUND cards. These three alternatives are represented in PyG4ometry with the BuiltIn, Material, and Compound classes. Populating a hierarchy of instances using these classes is made more involved due to the fact that recursively-defined materials in FLUKA input files need not be defined in a logical order. Namely, a given compound may be defined before the materials that it consists of are themselves defined. To account for this it is necessary to correctly compute the
instantiation order so that the above classes can be instantiated correctly. To do this a directed acyclic graph is populated with the materials and their constituents, after which a topological sort is performed so that the compound materials are sequenced after their constituents. Mapping this set of nested FLUKA materials to GDML materials is then straight forwards as the two formats are similarly expressive.

5.5. Lattice

FLUKA supports modular geometries with the use of the `LATTICE` command. Figure 6 demonstrates this capability. The arbitrarily complex `basic unit` can be defined once and used multiple times by placing one or more empty `lattice cells` with the associated rototranslation from that lattice cell to the basic unit. The lattice cells themselves will generally lack structure and simply serve as a reference to the basic unit. The rototranslated lattice cell must fully contain the basic unit and all of the regions within it. When a particle steps into the lattice cell, the rototranslation is applied to that particle transporting it to the basic unit, and the simulation continues. Any particles leaving the basic unit will be transported back to the lattice cell with the inverted rototranslation. Up to two levels of lattice nesting are supported in FLUKA.

![Figure 6: The lattice feature demonstrating a lattice cell referring to its basic unit with the rototranslation $R_{\text{trans}}$. Any particle entering the cell will be transformed onto the basic unit with $R_{\text{trans}}$, and when leaving the basic unit, back to the cell with $R_{\text{trans}}^{-1}$.](image-url)
This feature is clearly analogous to the logical/physical volume feature in Geant4, although it is more implicit as the contents of a given logical volume are explicitly stated, whereas the contents of a lattice cell are implied by the combination of the rototranslation and the global positions of its lattice cell and basic unit.

Translating the lattice construct into a logical volume (basic unit) with many physical volumes (lattice cells) requires associating each lattice cell with the full contents of its corresponding basic unit (typically more than one region). This is achieved by meshing the complete FLUKA geometry and then rototranslating the lattice cell mesh with its associated rototranslation. By construction this will translate the lattice cell mesh directly onto the full basic unit mesh. This transformed lattice cell mesh can then be intersected with all other meshes in the scene. Intersections with the transformed lattice cell mesh determine the contents of the basic unit. Finally, the contents of lattice cell can simply be replaced with a physical volume containing the logical volumes determined in the previous step. Thus a basic unit with one or more lattice cells can be translated into a Geant4 logical volume with one or more physical volumes. As has been stated, FLUKA supports two levels of lattice nesting, but currently the conversion to GDML supports only one. However, extending to an extra level is simple in that it only involves an additional application of a rototranslation matrix before checking for intersections with the lattice cell mesh. This capability will be added in a future release.

5.6. Discussion

Figure 5 shows a Faraday cup implemented in FLUKA and accurately translated to GDML using PYG4OMETRY. Many of the steps described above were directly applied in this model and all the features are tested and demonstrated in the repository. This set of algorithms for bridging FLUKA with GDML covers a very broad range of geometries, however a number of possible improvements remain for the future. For example, FLUKA regions can in general be disconnected, that is to say the resulting set of points defined by that region may consist of two disconnected subvolumes. In FLUKA this typically manifests itself in the form of a disconnected unions, but it is also allowed for intersections and subtractions to be disconnected. In the case of translating disconnected unions from FLUKA to GDML, this presents no difficulties as the GDML multi-union solid is explicitly allowed to be formed from disconnected parts. However, it is forbidden for Intersection
or Subtraction solids to be disconnected in this way and is therefore necessary to account for this difference between the two codes. One solution to this problem would involve detecting and separating disconnected meshes, and then placing each separated component as a separate TesselatedSolid instance. This decomposition has not been implemented and is left as future work.

Furthermore, the quadric surface conversion can be improved by specialising on some of the individual forms of the quadric. Simply converting every quadric into a TesselatedSolid comes at a potential performance cost in the tracking, as well as usability in PyG4ometry as the user must provide an AABB for every single region featuring a quadric body. In some cases tessellation is unavoidable (for example a hyperbolic paraboloid), but parabolic cylinders, for example, could be mapped to ExtrudedSolid instances. This could provide both a performance improvement in the tracking time and make PyG4OMETRY easier to use as an AABB would not need to be provided beforehand. This has not been implemented as quadrics are relatively rarely used, but where quadrics are used, it is often in the form of parabolic cylinders (e.g. magnet pole tips) and this specialisation in particular would be worth implementing.

6. GDML to FLUKA conversion

It is relatively straightforward to convert Geant4 geometry to FLUKA. Each of the Geant4 solids can be mapped to a FLUKA region. A region is a volume of space defined by a material and the Boolean disjunction (a union using the operator | in free format geometry, the most widely-used FLUKA CSG format) of one or more zones. Each zone is then defined in terms of the conjunction (intersection with +, subtraction with −) of one or more primitive bodies, as well as parentheses to determine the order of operations within the zone. FLUKA has 20 of these primitive bodies, listed in Table 1 and, in general, infinite-extent bodies have tracking accuracy and efficiency benefits over finite ones. Key for conversion are XY-, XZ-, YZ-Planes (XYP, XZP, YZP), arbitrary plane (PLA), Z-axis aligned cylinder (ZCC), Z-axis aligned elliptical cylinder (ZEC), sphere (SPH), truncated right-angle cone (TRC) and general quadric surface (QUA). Some solids in Geant4 directly map to a single FLUKA body, others require the construction of a simple FLUKA CSG tree combining these primitives. Table 6 lists the mapping between Geant4 solids and the bodies used to compose a FLUKA region.
Figure 7: Example conversion of a simple GDML geometry to FLUKA, above: the original model in PYG4ometry, below: the converted FLUKA geometry viewed in flair. The example is a sector bend dipole electromagnet.
| Geant4 solid | FLUKA region construction |
|-------------|---------------------------|
| Box         | +2 XYP + 2 XZP + 2 YZP   |
| Tube        | +ZCC - 2 PLA - 2 XYP - ZCC|
| CutTube     | +ZCC - 4 PLA - ZCC       |
| Cone        | +TRC - TRC - 2 PLA       |
| Para        | +6 PLA                   |
| Trd         | +6 PLA                   |
| Trap        | +6 PLA                   |
| Sphere      | +SPH - SPH - 2 PLA - 2 TRC|
| Orb         | +SPH                     |
| Torus       | +N ZCC - N PLA           |
| Polycone    | +N TRC - 2 PLA           |
| Polyhedra   | +N PLA                   |
| Eltube      | +ZEC - 2 XYP             |
| Ellipsoid   | +ELL - 2 XYP             |
| Elcone      | +QUA - 2 XYP             |
| Paraboloid  | +QUA - 2 XYP             |
| Hype        | +QUA - QUA - 2 XYP       |
| Tet         | +4 PLA                   |
| Xtru        | +N PLA                   |
| TwistedBox  | +N PLA                   |
| TwistedTtap | +N PLA                   |
| TwistedTrd  | +N PLA                   |
| TwistedTube | +N PLA                   |
| Arb8        | +N PLA                   |
| Tessellated | +N PLA                   |
| Union       | $R_1 \cup R_2$           |
| Subtraction | $R_1 - R_2$              |
| Intersection| $R_1 \cap R_2$           |
| MultiUnion  | $R_1 \cup R_2 \cup R_3 \cup$ |

Table 2: GDML/Geant4 solids and the mapping to FLUKA regions.

Understanding the algebra of FLUKA CSG and how it relates to Geant4’s concepts of solids, logical volumes and physical volumes is necessary to perform an accurate conversion. For example, a Geant4 logical volume solid may correspond to a FLUKA region consisting of many zones (i.e. unions), e.g., $R_1 = +z_1 \mid +z_2$. If this logical volume is placed as a physical volume in-
side some mother volume with its solid perhaps consisting of multiple zones, e.g., \( R_2 = +z_3 \mid +z_4 \), then subtracting a hole in the mother solid to make room for the daughter results in an equation of the form
\[
R_1 - R_2 = ( +z_1 \mid +z_2 ) - ( +z_3 \mid +z_4 ) = ( +z_1 - z_3 - z_4 ) \mid ( +z_2 - z_3 - z_4 ).
\]

(5)

Geant4 has Boolean solids associated with difference, union and intersection, so in addition to Equation 5, both \( R_1 \cup R_2 \) and \( R_1 \cap R_2 \) are required in FLUKA notation, so
\[
R_1 \cup R_2 = ( +z_1 \mid +z_2 ) \cup ( +z_3 \mid +z_4 ) = +z_1 \mid +z_2 \mid +z_3 \mid +z_4
\]
\[
R_1 \cap R_2 = ( +z_1 \mid +z_2 ) \cap ( +z_3 \mid +z_4 ) = +z_1 + z_3 \mid +z_1 + z_4 \mid +z_2 + z_3 \mid +z_2 + z_4.
\]

(6) (7)

Apart from the lattice feature, FLUKA has no sense of a volume hierarchy. Each body is placed with translation, rotation and expansion geometry directives in global coordinates. A transformation from world coordinates to a physical volume is built up by recursively applying daughter volume transformations and this is used to place FLUKA bodies. This in practice is very similar to the procedure to create the VTK visualisation already described in Section 3.2.

In FLUKA every single point in space needs to be associated with one and only one region. This presents a problem when converting Geant4 logical volumes to FLUKA regions, as the logical volume outer solid \( S_{\text{logical}} \) needs to have the daughter solids \( S_{\text{daughter},i} \) subtracted. A solid which can be converted to a region \( S_{\text{region}} \) is then
\[
S_{\text{region}} = S_{\text{logical}} - S_{\text{daughter},1} - S_{\text{daughter},2} - S_{\text{daughter},3} \ldots
\]
\[
(8)
\]

If a logical volume has a number of daughter volumes which are also possibly Boolean solids, then computing \( S_{\text{region}} \) can become very complex because of Equations 5, 6 and 7.

Figure 7 shows an example conversion from GDML to FLUKA. The example is a vacuum chamber with three ConFlat flange (CF) beam pipes connected to CF flanges. The top and bottom plates have been removed to display the geometry more clearly. The model is formed of Box, Tubs and Boolean operations of subtraction, intersection and union.
6.1. Non-convex solid decomposition

In general the BREP solids used in Geant4 include non-convex solids such as polycones, extrusion solids, and twisted solids. Converting these solids to an equivalent FLUKA representation is problematic as non-convex solids can only be created by the union of convex zones. Generating these zones is non-trivial and these solids can be divided into two groups based on the techniques required for the decomposition. First are those where only a 2D polygonal section needs to be decomposed, and these include polycones, polyhedrons and extrusion solids. The second group are those which require a full 3D convex decomposition, and these include the twisted and tessellated solids. This second group of non-convex solids are converted to CGAL Nef polyhedra [25] and decomposed to convex polyhedra [26].

6.2. Disjunctive normal form and degenerate surfaces

FLUKA will typically decompose a region into disjunctive normal form (DNF) at runtime, this normal form is characterised as the union of intersections and subtractions,

\[ R = z_1 \mid z_2 \mid z_3 \mid z_4 \ldots \]  

(9)

Defining regions in terms of the DNF allows the rapid test of whether a point is inside that region. Testing each zone \( z_i \) of \( R \) can terminate if a point is determined to be inside any of the zones \( z_i \). In general Equation 8 does not have the form of a DNF. If there are many levels of logical-physical volume placement, then recursive application of Equation 8 will create a nested set of parentheses. There are some conditions where a general Boolean expression can yield an exponential explosion of the final DNF. There are well known algorithms to convert logical expressions to its DNF. Pyg4ometry can simplify parentheses from a region by creating a corresponding SymPy [27] Boolean expression and using the to_dnf method. Further simplification of the CSG tree leverages Pyg4ometry’s meshing capabilities combined with CSG pruning algorithms based on [28]. FLUKA will by default try to expand all regions to their DNF at runtime, which inevitably can result in the sort of exponential explosion already mentioned. Until version 4.0, if FLUKA identified such an explosion, it would terminate the expansion, report an error and exit, thus making such models impossible to run. As of version 4.0, however, this expansion can be disabled, and the tracking algorithms will walk the CSG trees verbatim, albeit at some tracking efficiency cost.
Therefore, most output generated from the GDML to FLUKA conversion described here can only be used with FLUKA 4.0.

6.3. Materials

Pyg4ometry converts GDML/Geant4 materials to FLUKA MATERIAL and COMPOUND cards. Geant4 has a class G4Material to assign material state (density, physical state, temperature and pressure) to a logical volume. G4Material has two main constructors, the first where an atomic number is supplied and the second is when G4Element instances and relative atomic or mass abundances are provided. The simple G4Material is converted to a MATERIAL card, whilst the element G4Material is converted to a COMPOUND card. There are similar issues when converting G4Element to FLUKA, as G4Element can either be simple, i.e. defined only by atomic number and mass, or composite and defined by an admixture of relative abundances of isotopes. A similar mapping is performed so that if a G4Element is simple it is directly converted to a FLUKA MATERIAL card, and the isotope G4Element is converted to a COMPOUND card. Geant4 also defines a set of standard materials [29] or compounds from the US National Institute of Standards and Technology (NIST), so a user can, for example, simply specify the name G4_STAINLESS-STEEL. Pyg4ometry contains a matching database and creates the appropriate FLUKA cards from these names during the conversion. This database is updated when necessary by running a small Geant4 program to output the appropriate material data.

6.4. Discussion

Overall the conversion to FLUKA input format from GDML is quite advanced and stable. Relatively large experimental simulations have been converted from GDML to FLUKA and have been used to produce simulation results. The conversion described still requires a user to understand how geometry is specified in both Geant4 and FLUKA. For example, as has been stated, a Geant4 mother volume will, when translated to a FLUKA region, have all of its daughters subtracted from its respective FLUKA region. If those daughter volumes, when translated to FLUKA, consist of combinations of many FLUKA bodies, the mother region can become very complex. This complex region will generally not be in disjunctive normal form and is inefficient when viewed in FLUKA’s graphical user interface (GUI), flair, and used for simulation in FLUKA. Users who wish to minimise this should ensure that there are not large numbers of daughter volumes at the same level in
the hierarchy, unless corresponding to solids which translate to simple primitives such as boxes. Complex daughter volumes consisting of solids that are complex Booleans should be placed inside solids that map to primitive FLUKA bodies. This ensures that expanding to the DNF is computationally tractable, and in doing so FLUKA's tracking will be faster. This is not a drastic constraint on the conversion functionality, however, as this is actually typically how one would implement geometries in FLUKA regardless.

With the above in mind it is perhaps preferable for a user creating geometry from scratch to use Pyg4ometry and these conversion tools as part of the process. This would allow a user to target multiple codes with a single source description with minimal additional effort. However, there are still a number of outstanding technical issues with the conversion, which are discussed in the rest of this section.

Replica, division and parametrised placements are not currently implemented and will be added in a future release. In Geant4 it is possible to create scaled solids or placements with reflections (referred to as scale in Geant4). FLUKA rototranslations do not support reflections and implementing reflections requires transformation of the body definitions. This is not yet implemented in the current version of Pyg4ometry.

In general, recursive application of Equations 5, 6, 7 and 8 can result in very complex regions when converting from Geant4/GDML to FLUKA. The complexity of the final region expression can be compounded if transformed to DNF. The final region Boolean expression in DNF can be simplified by using the meshes of the intermediate parts, only retaining terms which do not contribute to the overall definition of the geometry (e.g. subtracting with a solid that does not overlap any other solid), using an algorithm similar to the one outlined in [28].

It is possible given the GDML to FLUKA conversion algorithm described in this paper that coplanar overlaps exist in the FLUKA geometry. In Geant4 there is no connection between surfaces used to specify one logical volume solid and another logical volume solid. For example if a logical volume solid shares a face with one its daughter volume solids, and those faces when translated to FLUKA are expressed in terms of half-spaces for example, those half-spaces would be duplicated in the final FLUKA file. It is possible to remove obvious degeneracies but this is complicated by placements of bodies. Every FLUKA body with an arbitrary number of associated transformations (rototranslations, rotations or expansions) provided by geometry directives can be re-expressed purely in terms of a body (possibly of a different type)
without any transform. A simple example of this is the XYP and PLA, it is simple to transform an XYP into a PLA with an appropriate rotation. This normal form can be used to test for approximate equality between bodies that are equivalent whilst accounting for any transforms. Approximate equality is required as multiple applications of rototranslations will accrue numerical rounding errors such that true equality is not maintained. This would allow for the removal of degenerate surfaces removing potential coplanar overlaps and also reduce the final converted file size.

The twisted primitive solids need to be decomposed into a union of convex solids. This decomposition does not always succeed or produces a far from optimal number of convex solids. An alternative to implementing these solids is to approximate each layer of the twisted solid as a union of tetrahedra. A similar problem exists for tessellated solids, which in general are non-convex and need decomposition into convex hulls. An alternative to the computationally expensive convex decomposition is to create a region formed from the unions of tetrahedra. There are numerous algorithms for tetrahedralisation of surface meshes in both CGAL and TetGen [30] and these will be implemented in a future release of PyG4ometry. Even if a stable and general method for converting tessellated solids exists, it is not efficient to define tessellated objects in this way. Memory, body or zone limits might be reached in FLUKA, thus possibly limiting the size of CAD or STL models which might be loaded.

7. STL and CAD to GDML conversion

STL and CAD conversion are closely related. In both cases the solid (in the case of STL) and solids (in the case of CAD) are converted to tessellated solid(s). STL is a relatively simple file format that can be loaded using pure Python. As STL files typically only contain a single solid the stl.Reader provides a single solid and not a logical volume as with the other file readers.

STEP and IGES files can be loaded into PyG4ometry, via an interface based on FreeCAD [7]. FreeCAD is an open source CAD/CAM program, which in turn is based on OpenCASCADE. FreeCAD allows for scripting in Python and acts as a simple-to-use interface to OpenCASCADE. A STEP CAD file could be considered as a hierarchical tree of parts and part assemblies, where a part assembly is a collection of part features. A part feature can be used to create a triangular mesh which can be used to instantiate
Figure 8: Example conversion of a simple CAD (STEP) geometry (sector bend dipole electromagnet) to GDML, above: the original model in FreeCAD, below: the GDML geometry viewed using PyG4ometry.
a PYG4OMETRY TessellatedSolid. The placement of the part feature is extracted from the STEP file and used to create an appropriate physical volume. Assignment of materials and visualisation attributes must be performed by the user after conversion to GDML as it is rarely the case that CAD/CAM packages include the detailed information required for MCRT codes. The loading of STEP files in PYG4OMETRY is demonstrated in Listing 4.

Listing 4: A simple PYG4OMETRY Python script to load a STEP file.

```python
import pyg4ometry.freecad as freecad

reader = freecad.Reader("CadFileName.step")
reader.relabelModel()
reader.convertFlat()

logical = reader.getRegistry().getWorldVolume()
```

Compared to other file readers, two additional steps are required: `relabelModel` and `convertFlat`. CAD model part names can contain characters which are not allowed in Python dictionaries so need to be replaced by using `relabelModel`. CAD models might also have a hierarchy of parts and assemblies, these are converted without this structure by using `convertFlat`. In general there is no requirement to avoid geometric overlap of parts in a CAD file. This will result in overlaps between the converted tessellated solids. This is avoided by shrinking each solid by computing the normal $\mathbf{n}$ for each vertex $\mathbf{v}$ and shifting its position by $\epsilon\mathbf{n}$, so that the new vertices are positioned at $\mathbf{v} - \epsilon\mathbf{n}$. The degree of shrinkage is user-controllable.

An example geometry representing a dipole electromagnet, consisting of three parts was created in Autodesk Fusion 360 and saved as a STEP file, the PYG4OMETRY-produced output is shown in Figure 8.

8. Complete simulation example

PYG4OMETRY is designed to be as flexible as possible and offer the user a wide range of usage styles, input files and workflows. A fictitious beamline was created to demonstrate the capabilities of PYG4OMETRY, this creates a composite scene which consists of geometry sources from the different formats described in this paper. The beamline consists of a vacuum chamber (modelled in PYG4OMETRY), a vacuum gate valve (STL from the manufacturer), a triplet of quadrupole magnets (exported to GDML from BDSIM),
Figure 9: Complete composite example using Pyg4ometry showing a model with geometry sourced from a range of different formats.

a sector bend dipole electromagnet (created in Autodesk Fusion 360) and finally a Faraday cup (FLUKA geometry designed in flair). Each different file is loaded using the appropriate Pyg4ometry Reader class and then placed as a physical volume. The final composite geometry is shown in Figure 9. It must be noted that when this complete geometry is written to GDML and loaded into Geant4 it cannot be visualised with anything but the ray tracer due to limitations in the OpenGL visualisation in Geant4. Another important note is that this geometry cannot be converted to FLUKA as it contains tessellated solids (both the STL gate valve and dipole magnet).

Having geometry wrapped in a suitable API allows a wide range of processes to be performed simply and programmatically. The benefits of the API are particularly apparent when needing to process large amounts of geometry efficiently and precisely. Possible transformations include merging registries, removing volumes (defeaturing), editing solid parameters, changing logical volume materials and converting logical volumes to assembly volumes.

The merging of registries and removing of volumes is required to create the example shown in Figure 9. Each sub-component is stored in a separate registry and these have to be combined without any GDML tags clashing. The FLUKA to GDML conversion creates logical volumes which are not generally required in Geant4, so for example the air surrounding the Faraday cup, which is needed to specify a FLUKA geometry is converted to GDML but can be safely removed. Examples of other workflows or geometry manipulation processes can be found in the Pyg4ometry online manual.
9. Quality assurance

The source and manual code for PyG4ometry is stored in a Git repository (https://bitbucket.org/jairhul/pyg4ometry), where a public issue tracker for users is hosted to report problems or bugs with the code. The Python source is documented throughout using docstrings, which are also used to generate an API reference using Sphinx, a Python documentation generator (http://www.pp.rhul.ac.uk/bdsim/pyg4ometry/). This automatically-generated documentation is supplemented with developer-written documentation in the form of examples and tutorials, again using Sphinx. PyG4ometry uses mature packages available for Python as dependencies. PyG4ometry has two sub-packages that require compilation: pyg4ometry.pycsg in Python and pyg4ometry.pycgal in C++. PyG4ometry package dependencies and extensions are easily installed using setuptools. All aspects of PyG4ometry are routinely checked using software tests, of which there were 543 at the time of writing, resulting in 84% code coverage. The tests also serve as minimal examples to help users understand the code operation.

10. Conclusions and discussion

The authors believe that tools to quickly create geometry, either from scratch or by conversion, for Monte Carlo particle transport programs will save significant amounts of time and user effort and will ultimately yield more accurate simulations. PyG4ometry is a relatively complete implementation of a geometry creation tool, and whilst heavily internally based on Geant4 and GDML, it can have utility for users of all MCRT codes. PyG4ometry can clearly be extended to other formats or applications. Presently it provides a coherent and uniform interface to existing tools and utilities, and by using the Python programming language the programmatic control of geometry creation or modification is possible. This approach allows the integration of other available tools [31] into a unified workflow.

Users should be aware of issues with PyG4ometry. The conversions between CAD/STL, GDML, and FLUKA cannot be considered bidirectional. For example, Geant4 tessellated solids cannot be converted easily to FLUKA which does not have a convenient way of representing this geometry. In general a user would be unwise to attempt to convert a very large geometry from one format to another, but should instead concentrate on smaller conversions.
of constituent parts, and then using those parts to supplement larger models. Workflows should focus on the generation of a primary format and then create conversions to other formats as the need arises. This paper outlines the creation of geometry using Pyg4ometry, and whilst that geometry is subsequently loaded into Geant4, flair and FLUKA, detailed studies of the MCRT simulation performance is beyond the scope of this publication and will be addressed in the future.

There are many output format extensions that can be considered for Pyg4ometry. Geant4 geometry is primarily created by writing C++ programs, so an output writer that converts the Pyg4ometry in-memory representation to C++ will allow rapid geometry modelling and inclusion of the geometry into an existing Geant4 application. This is not implemented in the current version but could be relatively quickly implemented for users that require this functionality. At present Pyg4ometry supports reading and writing Geant4 (GDML) and FLUKA files but could be extended without significant effort to other MCRT codes like MCNP.

There are more complex extensions that can be considered for inclusion into Pyg4ometry. The meshes created by Pyg4ometry are generally of very high quality and can be used for a wide range of applications. An idea already being developed is the export of the geometry mesh data to data formats used in augmented or virtual reality software to create interactive visualisations of MCRT simulations. Triangular meshes also have applications for GPU-accelerated photon tracking in optical photon based particle physics detectors. ParaView/VTK are becoming standard software for complex 3D visualisation and the ability to write geometry to formats readily loaded and manipulated by these programs will significantly aid the presentation of geometry along with the results of MCRT simulations.

Pyg4ometry is principally a toolkit but various visualisation and user interface extensions would significantly aid geometry creation workflows. A graphical user interface would enable a user without any programming experience to create geometry for MCRT simulations and expand the number of potential users. Pyg4ometry has been designed to interface with a GUI in a relatively straightforward manner. The VTK visualiser currently limits the display of very large models as geometry instances are replicated as opposed to reused in visualisation. However, this could be drastically improved in a future release.

The conversion which would most dramatically enhance the creation of MCRT geometry is CAD to Geant4 or FLUKA without use of a triangular or
tetrahedral mesh. There are existing approaches to decompose BREP solids to Geant4 and FLUKA-like CSG geometry [18, 32]. The FreeCAD/OpenCASCADE interface combined with the Geant4 and FLUKA Python API in Pyg4ometry will allow for the creation of CAD BREP decomposition algorithms. There are Python-based CAD modelling tools like CadQuery [33] which allow the creation of models using pure Python which should allow the conversion of GDML to STEP.

There is a strong relationship between Pyg4ometry and Geant4 and to a lesser extent between Pyg4ometry and FLUKA. Pyg4ometry can be used as a testing ground for ideas prior to implementation in Geant4 or FLUKA. An example of this is the VTK visualisation system implemented in Pyg4ometry, which could be used in Geant4 to render Boolean solids which frequently fail in the Geant4 OpenGL viewer, despite being otherwise perfectly valid constructs. This would involve using CGAL meshing in the G4Polyhedron class.

Pyg4ometry is already proving to be a useful tool for geometry conversion, creation and manipulation. There are numerous international researchers and research groups already using the code for their particular applications. The users are focused in accelerator physics, but Pyg4ometry could find application in any scientific area where MCRT simulations are needed, for example particle physics, space environment and medical physics. The authors welcome contributions, extensions and bug fixes as well as suggestions for larger collaborations.

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