Parallel Geometries in Geant4: foundation and recent enhancements

J. Apostolakis, M. Asai, G. Cosmo, A. Howard, V. Ivanchenko, M. Verderi.

Abstract— **The Geant4 software toolkit simulates the passage of particles through matter. It is utilized in high energy and nuclear physics experiments, in medical physics and space applications.**

For many applications it is necessary to measure particle fluxes and radiation doses in parts of the setup where there are complex structures. To undertake this in a flexible way, Geant4 has tools to create and use additional, parallel, geometrical hierarchies within a single application. A separate, parallel geometry can be used for each one amongst shower parameterization, event biasing, scoring of radiation, and/or the creation of hits in detailed readout structures. We describe the existing basic capabilities of the Geant4 toolkit to create multiple geometries and the recent major enhancements undertaken to streamline, enhance and extend these.

New functionality enables Geant4 developers to offer new embedded schemes for scoring (requiring no user C++ code); has simplified the implementation of processes or capabilities using alternative geometries. In addition they provide advanced users easy to use tools with which to create new processes or applications which use different (or common) geometries for any purpose.

I. Introduction

THE Geant4 simulation toolkit [1][2] provides comprehensive detector and physics modeling capabilities embedded in a flexible structure. It is in use by many high-energy physics experiments, projects in space science [3] and medical physics [4] to simulate setups of arbitrary complexity.

Key capabilities of this kernel include, geometry description and navigation, and tracking which interfaces with its physics processes and models.

This paper provides an overview of the capabilities of the Geant4 toolkit for creating and utilizing multiple geometrical descriptions of a setup. Their primary uses are for performance optimization, by parameterizing the energy deposition of showers or biasing the Monte Carlo to sample efficiently tracks in an important region[5], and for measuring the effects of the passage of particles, in scoring radiation dose and flux. New features that greatly enhance Geant4 toolkit's capabilities for parallel geometries are described in this paper, and have been publicly available since Geant4 version 9.0, released in June 2007, and improved in subsequent versions including Geant4 release 9.1 of December 2007.

The enhancements enable the use of biasing for charged particles in a magnetic field, provide standard ways to create and manage parallel geometries, and couple the parallel navigation consistently with Geant4 kernel classes, including the tracking.

II. Parallel Geometries : Foundation, established uses and limitations

The new capability has been built on top of the existing ability to create independent geometries for different potential uses and exploits the existing enhanced interface provided by the navigation system in the Geant4 toolkit [1]. A geometry setup is in general associated in Geant4 to a specialized *navigator* concrete instance of a *G4Navigator* class. The *G4Navigator* has been designed in such a way that several instances of it can be created and coexist, being assigned different roles. The main navigation system is attached to the geometry in which the material of a setup is described; this setup is unique, and is used for all physical interactions; we refer to it as the 'mass' geometry. Other navigator objects can be assigned to the same geometry and be used for example as simple 'locators', independent from the actual tracking, to identify exact positioning in the mass geometry of a particular point in the global coordinates system.

The capability to have alternative (*parallel*) geometries is enabled by the structure of the Geant4 geometry [6] and toolkit. Each geometry must have an independent root volume (the *world* volume), which contains a hierarchy of physical volumes. For the simpler geometry models more than one navigator object can be assigned to each geometry and perform operations independently.

Once a user has created a geometry, it is necessary to create a *G4Navigator* object to assign to it, in order to locate points and calculate the linear distance to the next boundary. This geometry can be associated with the read-out structure of a detector, with a simplified description of a setup such as a calorimeter for use in shower parameterization or for use in 'importance biasing' or scoring of doses and other radiation measures.

These basic capabilities have been available in the Geant4 toolkit since several years, and exploited for applications in HEP, including the BaBar experiment for fast simulation uses.

The existing approach was however exposed to several limitations. The information about the location of a track in the mass geometry was not propagated by the Geant4 kernel to potential parallel geometries and vice-versa; as a result of this,

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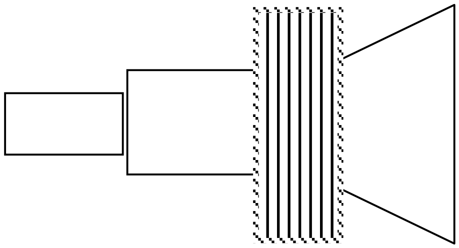

Figure 1. Picture of a simple setup with 2 parallel geometries: the 'material' geometry of two boxes and a trap overlaid by the mesh for scoring radiation flux. The scoring geometry must be separate and parallel, as it occupies the same space. Otherwise it would cause overlap errors.

each process requiring a parallel geometry had to undertake significant book-keeping, including the task of initializing the location for each new track. In particular, the implementation of those processes applicable to either a parallel or mass geometry was rather complex and inefficient.

The transportation (*G4Transportation*) process in Geant4 is responsible for identifying the next boundary, applying the effects of an external electromagnetic field and transporting the particle in the geometry setup, taking into account limitations to the step by physics processes. In its original design, *G4Transportation* used not to take into account of the presence of alternative geometries and the contribution that these could give for limiting the step. As a result, the curved path of a charged particle in an electro-magnetic field was calculated and its intersection was found only considering the boundaries of the mass geometry. In the case of fast simulation, for instance, some extra work was required by additional processes for triggering shower parameterization, recreate this curved path and intersect it independently with its alternative (*ghost*) geometry. In addition, this approach was exposed to inaccuracies in the calculation of the final endpoint of a step, particularly in presence of magnetic field and charged particles; a process which moved the endpoint of a step could not have full information about the maximum safe distance, unless all processes reported an accurate isotropic safety distance for the endpoint corresponding to their alternative geometry.

Due to these limitations, it was challenging for an advanced user to create an application with one or several alternative geometries and several restrictions had to be considered.

III. New Capabilities

In order to resolve the limitations imposed in the old approach, several enhancements have been provided. A new standard way to create a parallel geometry was conceived and provided the ability to activate each parallel geometry independently, depending on the type of particle.

The user can define more than one parallel geometries simultaneously. In a parallel world, the user can define arbitrary volumes, making them sensitive, or assigning regions, shower parameterization setups, and/or importance weights for biasing. Volumes in different parallel geometries can overlap. The revised *G4Transportation* process will become automatically aware of the presence of multiple geometries and will be activated only after the registration of the parallel geometry in the detector description setup.

The class *G4TransportationManager* provides all the utilities to retrieve, activate and verify the navigators associated to the various parallel geometries defined.
A new abstract base class, *G4VUserParallelWorld*, has been provided and should be adopted by the user, implementing in a derived class the appropriate *Construct()* method, where the setup for the parallel geometry should be defined. The root world volume assigned to the parallel geometry must have a unique name, and should be set as an argument to the class constructor; it will be automatically created by *G4RunManager* as a clone of the mass geometry world volume, at the time the geometry gets registered. The *Construct()* method provides as return argument the pointer to the cloned world physical volume generated; the pointer can also be accessed through the *GetWorld()* method defined in *G4VUserParallelWorld*. The volume hierarchy of the parallel geometry can be defined in the traditional way and provided to the generated world volume.

The new implementation allows different processes to optionally share a parallel geometry in a transparent way. A new class (*G4PathFinder*) polls all active geometries to identify the location of a point and to identify the next boundary along a linear or curved trajectory.

Each existing or new capability that requires an alternative geometry must message the *G4PathFinder*. Typically it will require a Geant4 Process, which will be polled at each step by the tracking engine. In turn it must message *G4PathFinder*, to find whether its geometry has the shortest distance to the next boundary.

Particular attention is paid to the coupling of the geometry to the electromagnetic processes, and in particular to the multiple scattering process. Electromagnetic processes [7] [8] utilize the isotropic safety, which is an estimate of the distance to a boundary in any direction. The ionization process uses this quantity in particular, in order to enhance the production of delta electrons. A sample of delta electrons with range large enough to reach the nearest surface are emitted - when the option of 'sub-cutoff' is set.

In addition, the Geant4 multiple scattering process [9] utilizes the isotropic safety to limit the lateral displacement it applies at the end of step. A lateral displacement larger than the safety is reduced to the size of the safety (as a result for steps that end on a boundary, where the safety is zero, the multiple scattering does not apply a lateral displacement**).**

A new class, *G4SafetyHelper* streamlines communicating with electromagnetic classes, including the Multiple Scattering. For efficiency it caches the values of the safety for the material geometry and of the minimum safety over all geometries. This object also knows whether a simulation is running in simple or coupled mode, and acts accordingly. It can communicate either to the active Navigator (in simple mode) or to the PathFinder (in coupled mode.)

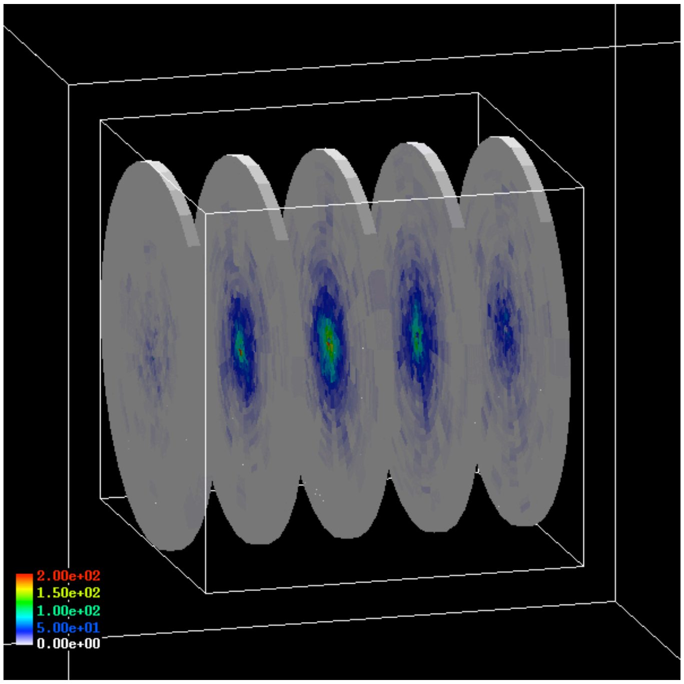

Figure 2. Example of a cylindrical scoring geometry embedded inside a large water volume. The scoring geometry is created at run-time, in a separate parallel geometry. No checking for overlaps with the 'material' geometry is required as a consequence.

It has extra two interfaces: the first allows one selected process to relocate the track; the second obtains the estimate of the linear distance to the next geometry boundary. The first interface is used by the multiple scattering processes when it samples a displacement of the end point of the step due to scattering. Second is utilized by optional step limitation algorithm applicable for setup without magnetic field.

The information about safety is used by the ionization process, to enhance the production of delta electrons when the option of 'sub-cutoff' is set [7]. For that at each step of the track the value of geometrical safety is compared with the cut in range for delta-electrons for the given media. Near the boundary the lower value of the cut is used. This feature allows more efficiently simulate a transfer leakage of delta-electrons when high energy track is parallel to the volume surface.

The current implementation of the *G4SafetyHelper* takes into account possible existence of parallel geometry and allows multiple access from different electromagnetic processes to geometry information without significant CPU penalty.

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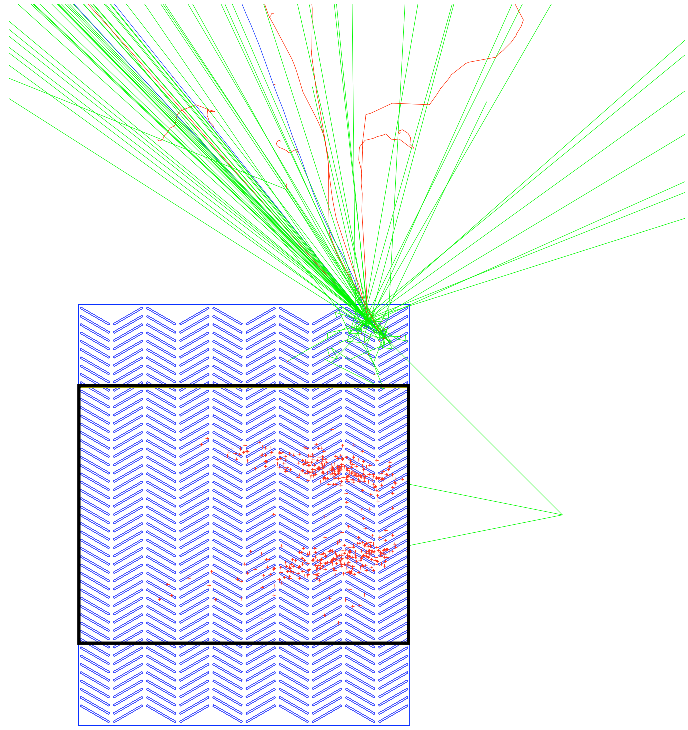

Figure 3. Example of utilizing a 'ghost' envelope volume for triggering a shower parameterization. The envelope is outlined by the black line, and belongs to a parallel geometry. It overlaps the complex, accordion-like structure of the calorimeter. Inside this envelope, the parameterization deposits sampled hits. Outside the envelope, full tracking is undertaken. The new developments have extended this ability, enabling its use when electromagnetic fields are present and simplified its implementation.

IV. Impact and Applications

The enhancements have enabled Geant4 developers to offer new embedded schemes for scoring (requiring no user C++ code). In addition they have simplified the implementation of processes or capabilities using alternative geometries. Also they enable advanced users to create applications using different geometries for scoring, event biasing and other abilities. Geometries can also be shared, for example using the same geometry for biasing and scoring.

The new framework allows the possibility to importance bias all particle types, including charged. Previously this was forbidden due to restrictions on parallel boundaries and multiple scattering. The new management of boundaries allows all processes to see boundaries in all geometries, which obviates the difficulties associated with multiple scattering causing a particle to scatter back whilst on an importance boundary.

As a result a key utilization of the new scheme for parallel geometries has been in enabling importance biasing and scoring in the presence of an electro-magnetic field.

In addition a new capability has been created for scoring common physics quantities, such as doses and fluxes, on rectangular or cylindrical meshes placed in arbitrary locations.

This scoring can be enabled without changes in C++ source code. It can be configured by text commands issued at run-time or stored in input files.

The fast simulation capability of Geant4 is now able to freely define ‘envelopes’, the volumes in which the user's shower parameterization can be triggered. As an example, in a complicated geometry of a HEP sampling calorimeter an envelope can be defined without concerns for overlaps. It can overlay a (parallel) 'ghost' volume encompassing the regular part of the calorimeter. In this part the shower parameterization is relevant. The envelope can leave out the parts of the modules near the boundaries. As a result detailed simulation will take place in these parts. All the different volumes and material of the calorimeter geometry are seen by the physics processes, but only the simpler envelope is required for the ghost volume.

V. Conclusion

New capabilities have been added to Geant4, in order to provide application creator with a standard way to create alternative geometries, and process writers with simpler ways to utilize these. The Geant4 Kernel has been enhanced to enable the navigation in parallel in all active geometries, consistently and transparently. As a result creating an application with an additional geometry for scoring radiation fluxes on arbitrary meshes has been made simple, In addition the ability to create several parallel geometries and to use in conjunction with other key features of Geant4, including tracking in a magnetic field, is streamlined and enhanced.

VI. Acknowledgments

We express our appreciation for the wealth and depth of feedback provided by Geant4 users, which has helped greatly in improving the toolkit and validating it for diverse use cases. We acknowledge the efforts our fellow Geant4 developers, who create and maintain many related aspects of the toolkit and have indirectly enabled these developments.

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