GEANT4: STATUS AND RECENT DEVELOPMENTS

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Abstract

Geant4 is relied upon in production for an increasing number of HEP experiments and for applications in many fields. Its capabilities continue to be extended, as its performance and modeling are enhanced.

An overview of recent developments in diverse areas of the toolkit is discussed. These include, amongst others, performance optimization for complex setups using production thresholds in different geometrical regions, improvements for the propagation in fields, new options for event biasing and an overview of additions and improvements in the physics processes. The progress in physics performance have benefited from the extensive physics comparisons and the validation effort undertaken in collaboration with a number of experiments, groups and users.

INTRODUCTION

The Geant4 toolkit [1] provides comprehensive physics modeling embedded in a flexible structure. The choice of physics modeling and the functionality of a robust kernel enable users to adapt its capabilities for diverse applications. This note provides a short update on developments undertaken by the Geant4 Collaboration [2] since March 2003.

The Geant4 kernel provides tracking, geometry description and navigation, abstract interfaces to physics processes, material description, management of events, run configuration, stacking for track prioritization, a framework for the creation of hits and digitization, and interfaces to external frameworks and GUI.

Physics processes included cover diverse interactions, and are organized as electromagnetic (EM), hadronic and decay processes. Particles tracked include leptons, mesons, hadrons and photons. Photons of optical wavelengths are for are treated by separate processes. Different implementations of physics process are offered in several energy ranges for many physical processes. These typically use complementary modeling approaches.

For each established application area, a set of physics simulation engines is provided. Each package is a configuration of physics processes (a 'physics list') that is tailored to address the specific requirements for accuracy in the most relevant physics observables, with varying levels of CPU resources.

In addition Geant4 provides interfaces to enable the users to interact with their application, and save their results. Visualization drivers and interfaces, Graphical User Interfaces (GUI)s and a flexible framework for persistency are included.

In order to meet the computing requirements of shielding and other applications, standard efficiency-enhancing techniques have been built into the toolkit. Variance reduction (event biasing) techniques and a framework for fast simulation (shower parameterization) are provided.

CURRENT DEVELOPMENTS

Geant4 5.0 (December 2002) included improved importance biasing & scoring, the first release of implementations of the Binary Cascade [3] and an implementation of the Bertini cascade [4], providing new theoretical hadronic models for energies between hundreds of MeV and about ten GeV.

The key feature of release 5.1 was the addition of the new ability to define geometrical regions, and set a different value for the production threshold (or cut) of photons, positrons and electrons in each region (cuts per region functionality).

Geant4 release 5.2 (June 2003) provided several refinements and additional capabilities, including improvements in the cuts per region functionality (EM refinements for performance and the saving and retrieving of physics tables), a performance optimization of the module for propagation of charged particles in a field and a revisions of the pion reaction cross-sections.

The focus of the releases in the past year (6.0 to 6.2) has been to provide further refinements, improvements, fixes for outstanding and new issues, performance enhancement and additional developments.

A key feature of release 6.0 was the use of a new implementation of electromagnetic (EM) processes as the default. The release included also, for the first time, the configurations of hadronic physics processes ('physics lists'). Further physics models and new functionality were provided. We note that a number of revisions required interface changes in user code.

A consolidation release (6.1, March 2004) provided a number of improvements to enhance stability for production, and new tools to identify infrequent problems. Relatively infrequent problems can have significant impact during large scale productions yet also occur on occasion in less intensive, general use. The most recent release (6.2, June 2004) [5] includes improvements and further new hadronic models.

THE KERNEL

This section examines new developments and improvements in the modules for geometry, particles, materials, tracking and run & event management. In addition it summarises the new options for variance reduction.

Geometry

A significant new feature in the Geometry is the abstraction of G4Navigator. This enables a user (either an application developer or a toolkit developer) to replace, change or add to the current Geant4 navigator. In addition a first consolidation simplifies the navigator interface.

New 'division' volumes were created that subdivide larger volumes, which extend the existing capabilities of 'replicas' by providing offsets. All Constructed Solid Geometry (CSG) volumes, including boxes, tubes, cones, and polyhedra, can be sliced along an appropriate axis, which is usually a symmetry axis.

The divisions are implemented in terms of existing parameterised volumes, and thus can be visualized better in the case of radial slicing than existing replicas.

Improvements to solids focused on a revision of 'isotropic safety', the estimated distance to the nearest volume boundary from the current point. The solids affected included the simple (CSG) solids and the Boolean solids, which are created using Boolean operations of other volumes – starting from CSG solids. Feedback from use in recent extensive tests and productions [6] assisted greatly in optimizing the implementation of the 'safety'. In addition a new solid, the G4Orb, addresses uses cases for a 'full' sphere, enabling the modelling of spheres of large dimension, e.g. one the size of a planet.

The GDML geometry description language [8] and it's module for interfacing with Geant4 have been extended. A new module enables a user to save an Geant4 geometries, which is in memory, by writing it into a XML text file. Support for more solids and for replicas has been added.

In addition a logical reorganization and restructure of sub-modules of the geometry was undertaken, together with a code review to reduce internal dependencies.

A major challenge in creating a new application is the need to create a 'correct' description of the geometry of the setup. For all geometries but the simplest, it is unfortunately easy to create overlapping volumes. Thus it is necessary to identify overlaps and enable the user to check whether one or more problems exists in a user's model geometry. Such problems or issues in navigating through a prototype setup typically arise due to an incorrect geometry description – yet on occasion can occur due to a limitation or problem in the G4Navigator implementation. In the recent past, new checks at geometry construction time have been introduced to ensure that the user create a geometry that respects Geant4's volume rules and limitations. An example rule is that simple 'placement' volumes cannot be placed inside a volume that is sliced in a replica or filled with a parameterised volume.

During tracking Geant4 does not check for malformed geometries – for reasons of performance & simplicity. In the latest releases a new option enables some checks of the user's geometry and the navigation during tracking. When using this geometry 'check' mode, Geant4 provides information on candidate intersections with volume boundaries to help users or developers to identify an underlying problem.

The full challenge of detecting 'significant' overlaps is addressed by specialized tools. These include the DAVID tool which intersects graphics volumes [9], an example program using the full Geant4 tracking / navigation [10] and a verification sub-module inside the geometry [11]. All these tools have adjustable intersection tolerances. The verification sub-module can run different verification tests and is accessible in any interactive Geant4 application through User Interface (UI) commands. Enhancements now enable its use on a sub-tree up to a specified depth, instead of a full geometry or full sub-tree.

Propagation in field

Charged particles in Geant4 are tracked in external electromagnetic fields, and the intersection of their curved trajectory with geometry boundaries is approximated to a user specified precision.

This module now provides the ability to specialize integration accuracy parameters for each Field-Manager. Another new capability enables the user to select, utilizing a track's properties, the accuracy parameters for tracking in field. This functionality enables a user, for example, to undertake precise tracking for all muons or for any tracks with energy above 5 GeV, while tracking electrons in a calorimeter more coarsely. Additional tests led to improvements in identifying and refining volume intersections.

To avoid unnecessary navigation sub-steps, the safety is used in tracking in fields. Potentially costly boundary intersections are avoided.

Run & Event

A redesign of the Run Manager module was undertaken, separating into a new class that functionality which is mandatory for the kernel. This refinement enables an experiment, or other advanced user, to create more easily a customized run-manager, which fits into its framework, yet is compact and easy to maintain. In addition the run manager now handles directly HEPMC events and track vectors, and can merge different sources of primaries.

In order to improve the link between a primary particle its pre-assigned decay products, the trajectories of all resulting tracks and their associated hits, new hooks for user 'helper' classes were created. These optional 'helpers' can carry user information for a primary vertex, a primary particle, an event or a region.

A significant design iteration of the General Particle Source class provided a new formula for converting integral spectrum to differential one, better interactivity and other improvements [13]

Variance reduction

Advanced developers have utilized event biasing in their Geant4 applications for some time, using user code. Since release 4.1 (June 2002), general-purpose biasing methods have been available in the toolkit. A module has provided importance biasing, with splitting and Russian roulette An importance value is associated with each volume. Either the 'mass' geometry (used for physics and tracking) or in a dedicated 'parallel' artificial geometry can be used for biasing. As expected, many applications, including shielding studies, experience large gains in time efficiency.

Capabilities added over the past 18 months include an implementation of the weight-window method, and of related but simpler 'weight-cutoff' method. Leading particle and cross-section biasing are provided for hadronic processes in the hadronic framework.

PHYSICS

Physics use cases

The Geant4 toolkit offers a variety of physics processes and model options for almost every energy range and interaction type. It is possible to choose many different configurations of models, in order to address the needs of a particular use case. Yet this freedom can create a daunting learning curve to obtain suitable physics choices.

To address this need, and to provide users with suitable choices, a set of use cases was identified [14]. For each use case a few packages or 'educated-guess' physics lists were chosen or created. An 'educated-guess' physics list can be used directly or treated as a starting point for creating a tailored configuration of physics processes and models. Currently nineteen use cases are covered by twenty-four physics lists.

Hadronic use cases relevant to HEP applications include HEP calorimeters, HEP trackers, a 'typical' general-purpose HEP detector, low energy dosimeter applications with neutrons, and low energy nucleon penetration shielding. In addition three use cases for electromagnetic physics were identified, and corresponding physics lists have been created.

Pre-packaged and versioned physics lists facilitate the comparison of physics results between different detector groups and the further specialization of the parts that vary most. Revisions, motivated by experience and benefiting from the many available comparisons [15] with data, have provided for improvements in a number of observables.

Electromagnetic Physics

A number of developments and improvements have been made in the Electro-Magnetic (EM) processes [16]. The module of traditional electromagnetic physics processes ('standard' EM), which are optimised for use in HEP detectors, has been refactored. This new version has been made the default since Geant4 release 6.0.

The new implementation is based on a "model-based" design, which simplifies maintenance and enables easier extensions and refinements. This implementation has kept user code unchanged. For a transition period the previous implementation has been available. Issues were encountered in the transition were addressed in patches and release 6.1.

Refinements include improvements to the tail of the angular distribution for multiple scattering, and improved calculation of the radiative corrections for the Bethe-Bloch model for muon energies above 1 GeV. A revision of multiple scattering ensure reproducibility in the presence of diverse ions.

In optical processes a new process implements wavelength shifting, and a revision improves the handling of surface properties for material interfaces.

New developments in low-energy EM physics include new high-precision models (2BN, 2BS) for the angular distribution of Bremstrahlung photons from incident electron energies below 500 keV [17], new processes implementing models from the Penelope [18] Monte Carlo program for electrons and positrons [19]

A large number of comparisons of physics observables between test beam (or experiments) and their simulations using Geant4 have extended the set of available validations [20].

Hadronic Physics

Two forms of biasing were added in the hadronic framework. The first enables leading particle biasing for any reaction, and the second provides cross-section biasing for electron-nuclear and gamma-nuclear reactions.

The Binary Cascade[3] now includes pion projectiles and light ion reactions and an improved transition [21] to pre-equilibrium model. The applicability of the implementation of the Bertini Cascade [22] was extended up to 10 GeV, and its suitability for isotope production estimation was verified.

The selection of the element undergoing an interaction, in preparation for creating final state has been improved. In addition, the choice of an isotope is now made centrally, before calling the models that create the final state. These improvements enable the use of models that can treat specific nuclei, especially those far from equilibrium.

New models for ion reactions include an implementation of Wilson's abrasion model [23] for ion-induced reactions and electromagnetic dissociation for ion-ion collisions [24, 25].

New models for the evaporation phase were implemented, including an ablation model [24] for use with abrasion and a new implementation broadly similar to the GEM model [26]. A new, alternative, set of emission probabilities has been added, taken from HETC [27], for Weisskopf-Ewing evaporation.

A new theory-based coherent-elastic model [28] utilizes pre-processed tabulations for elastic scattering. Also available are new implementations of muon nuclear absorption, of an improved fast radioactive decay and new, alternative, GNASH2 transition probabilities in the exciton pre-compound model.

A new technical development was undertaken to help solve issues reported by users. When a problem occurs during a program run, this identifies the initial conditions. A new white-board, a signal handler and use of C++ exceptions enable the module to record initial conditions of reactions and print them out in case of 'soft' errors or program crashes. As a result the turnaround time required to identify and resolve issues has been cut by an order of magnitude.

To aid in event reconstruction, a particle surviving a hadronic interaction can be relabeled optionally as a new particle. Improvements to cross sections include pion scattering data of Barashenkov, which remove existing discontinuities. A legacy problem in high energy p-H cross-sections was solved.

For ion-ion cross-sections improvements include an implementation of Tripathi's systematics for light ions and parameterizations from Shiver, Kox and Shen [29]. Improvements in the scattering term extended its use for nucleon induced reactions up to 8 GeV. S-wave absorption of pions and pion induced reactions up to 1.5 GeV were added. This energy is the limit for this approach, due to current knowledge of strong resonances.

REMARKS

Continuous checking is undertaken of computing time to monitor CPU performance. Benchmark applications include simple setups, test beam and a use case with a complex magnetic field.

The interaction with Geant4 users is providing very valuable feedback. A new method for discussing key issues with users has been instituted in the past year: the Geant4 Technical Forum is open to all interested parties and individuals, and meets quarterly to discuss technical matters, including identifying issues and weighing priorities. Developers continue to emphasize identifying problems, and providing assistance to users in using Geant4 for established and new use cases.

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We express also our appreciation of the wealth and depth of feedback provided by Geant4 users, which has been indispensable for improving the toolkit and in validating it for diverse use cases.

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