Recent developments in Geant4

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Abstract

Geant4 is a toolkit for simulating the passage of particles through matter and it is used by a large number of experiments and projects in a variety of application domains, including high energy physics, astrophysics and space science, medical physics and radiation protection. An overview of the physics processes in the toolkit is presented focusing on hadron interactions. The toolkit also has many other useful functionalities for shielding calculations. These include event biasing options and primitive scoring which provide an easy interface to simulation results.

Introduction

Recent high energy physics experiments require large-scale, accurate and comprehensive simulations of their detectors. Similar requirements also arise in other fields, such as astrophysics, space science and engineering, radiological sciences, radiation therapies and radiation protection research. Geant4 has been developed in order to satisfy such demands [1,2]. It is an object-oriented simulation toolkit which provides a variety of software components for users who want to simulate the response of their detectors. It can be used to simulate single purpose, basic and relatively simple detectors as well as the large, general purpose detectors used in modern, high energy physics experiments such as those at the Large Hadron Collider (LHC). Geant4 provides all aspects of the simulation process, such as:

1. geometry description;
2. material specification;
3. particle definitions;
4. tracking and navigation;
5. physics processes to handle the interactions of particles with materials;
6. management of events;
7. run configuration;
8. stacking for track prioritisation;
9. tools for handling the detector response;
10. interfaces to external frameworks, graphics and user interface systems.

Geant4 has abundant physics processes and models covering a wide energy range from optical photons and thermal neutrons to the high energy reactions at the LHC and in cosmic ray experiments. In addition to these processes and models, Geant4 also provides abstract interfaces to physics processes. Users are easily able to add their own physics models with these interfaces. The above features reflect the choice by Geant4 to adopt object-oriented technology and to follow an iterative-incremental software process [3]. This technology makes possible many extensions and improvements of the toolkit with no modification of the existing code. Because Geant4 is a toolkit, many users can incorporate Geant4 into their own simulation framework. However it can also be used to build a stand-alone application, in which a user defines his/her problems, executes simulations, gets results and creates graphics for presentations. Geant4 has been widely used in high-energy physics domains since its first release in 1999, and its use in many other fields of science has also increased. Radiation protection research is one such field.

In this paper, we provide an overview of the toolkit capabilities, focusing on topics related to shielding calculations. In the next section we give a brief review of Geant4 physics processes, excluding hadronic processes which will be covered in detail in another section. Selected functionalities useful for shielding calculations will be introduced in the following section. Finally we give a short summary.

Geant4 physics processes

Geant4 has abundant physics possesses for handling interactions of gammas (including X-rays and optical photons), electrons and positrons, muons, hadrons and ions. Before explaining these processes we briefly describe the particles and materials categories of Geant4 because the physics processes depend on their properties for the simulation of particle-matter interactions.

Particles

Geant4 provides most of the particles listed by the Particle Data Group [4]. Ions can also be defined with excitation energy and charge state. These Geant4 particles are created according to the following procedure:

1. A particle definition base class is provided which describes the basic properties of a particle, such as mass, charge and so on.
2. Virtual intermediate classes for leptons, bosons, mesons, baryons, etc. are provided in order to abstract particle properties common to these types.
3. A concrete particle class is derived which has properties specific to the particle.

Users who wish to create particles not already provided by Geant4 may do so by following the above procedure. The particle class has the list of physics processes to which the particle is sensitive.

Materials

In Geant4 materials are made of a single element or a mixture of elements, and elements are made of a single isotope or a mixture of isotopes. When a user needs water in his/her geometry, then he/she must first create the elements of hydrogen and oxygen. If heavy water is required in the simulation, the isotope deuterium must be created before defining the element hydrogen. Characteristics like radiation and interaction length, excitation energy loss, coefficients in the Bethe-Bloch formula, shell correction factors, etc., are computed from the element, and if necessary, the isotope composition. Users can change these properties. Geant4 also provides pre-defined materials whose properties follow the data library of the National Institute of Standards and Technology [5].

Processes

All physics processes must describe the interaction of particles with matter in a unified manner which is well-defined by object-oriented programming technology. Therefore all physics processes can be treated in the same manner as the other components of the simulation such as tracking. This means that the tracking code is completely general and common to all processes of all particle types. This provides flexibility in the design of a physics process, and together with the modular architectural framework, makes possible the development of new models without affecting existing code.

It is useful to divide the functionality of a process into two parts. One part manages when and/or where the interaction occurs and the other decides what occurs in the interaction. The former usually relates to the cross-section or mean-lifetime and the latter generates the final state. In many Geant4 physics processes, the two parts are implemented separately. In such processes it is possible to have multiple final state generators as well as multiple cross-section data sets.

Geant4 physics processes are divided for convenience into seven categories: electromagnetic, hadronic, transportation, decay, optical, photo-lepton_hadron, parameterisation. The electromagnetic and hadronic categories are further sub-divided. In this section we give a brief description of all of these except for hadronic. As the hadronic processes are of greatest relevance to shielding calculations, they will be treated separately in later sections.

Electromagnetic

Physics processes in this category handle the electromagnetic interactions of leptons, photons, hadrons and ions. Geant4 provides physics processes of ionisation, bremsstrahlung, multiple scattering, Compton and Rayleigh scattering, photo-electric effect, pair conversion, annihilation, synchrotron and transition radiation, scintillation, refraction, reflection, absorption and Cherenkov effect. For some of these processes there are multiple physics models which may be used to implement the interactions. This category is divided into *standard* and *low energy* electromagnetic processes.

Standard electromagnetic processes assume the following things: the projectile energy is more than 1 keV, the atomic electrons are quasi-free, that is, their binding energy is neglected except for some corrections at low energy, and the atomic nucleus is fixed, that is, the recoil momentum is neglected. Standard processes include Compton scattering, gamma-conversion into electron and muon pairs [6] and the photo-electric effect for photons.

Electron/positron bremsstrahlung, ionisation and delta-ray production, positron annihilation and synchrotron radiation are also included. Muon processes handle bremsstrahlung, ionisation and delta-ray production and electron-positron pair production. There are also ionisation processes with the production of delta-rays for charged hadrons and ions. The energy losses of charged particles are computed taking fluctuations into account. The default fluctuation model is Landau-like with additional Poisson-like fluctuations for soft energy transfers. An alternative model based on Photo-Absorption Interaction (PAI) [7] is also available. The multiple scattering process of Geant4 [8] can handle all charged particles. It does not use the Moliere formalism but is based on the more complete Lewis theory [9]. It simulates the scattering of the particle after a given step, computes the path length correction and the mean lateral displacement. The correlation between direction change and lateral displacement is included.

Low energy electromagnetic processes [10] are implemented in Geant4 in order to extend the validity range of electromagnetic interactions below 1 keV and the current implementation of its electron and photon processes can be used down to 250 eV. The low energy package includes the photoelectric effect, Compton scattering, Rayleigh scattering and polarised Rayleigh scattering, bremsstrahlung, and ionisation. The gamma conversion process has also been implemented. Fluorescence emission from excited atoms can be generated as well as Auger electrons. The implementation of electron and gamma processes is based on evaluated data libraries (EPDL97 [11], EEDL [12] and EADL [13]) that provide data for the determination of cross-sections and the sampling of the final state. Proton induced X-ray emission (PIXE) [14] is also available. Moreover there is an additional set of processes for photons, electrons and positrons in the low energy package. These processes are based on the physics models developed for the PENELOPE code (PENetration and Energy LOss of Positrons and Electrons) [15]. These implementations also provide reliable results for energies down to a few hundred eV.

The low energy electromagnetic processes are well-designed for being able to handle multiple models in a process. For example, the hadron and ion ionisation process of the low energy package adopts different models depending on the energy range. In the high energy (>2 MeV) domain the Bethe-Bloch formula [16] is used and in the low energy domain (<1 keV for protons) the free electron gas model [17] is used. In the intermediate energy range parameterised models based on experimental data from the Ziegler [18] and ICRU [19] models are implemented. The molecular structure of materials [20] and the nuclear stopping power [21] are taken into account.

Decay

At rest and in flight decays of particles are supported. Default decay tables for most unstable particles such as mesons, hyperons and resonant baryons based on data from the Particle Data Group [4], are provided. Decay modes are sampled according to the branching ratios in the particle's decay table. It is also possible for users to set the proper decay time and decay mode of the primary particle. There are many models for determining the distribution of daughter particles, for example V-A theory for muon decay, Dalitz theory for p0 decay, or simple phase space decay. Decay of radioactive nuclei is also supported and data tables derived from the Evaluated Nuclear Structure Data Files [6] are prepared for over two thousand nuclei. However radioactive decay is currently classified as a hadronic process in Geant4.

Transportation

In Geant4, transportation is also treated as a kind of physics process. The transportation process propagates a particle through a detector geometry in the presence of magnetic or other fields and guarantees that steps within particle trajectories end at geometrical boundaries. Users may also set the maximum length of a single step.

Optical

Geant4 can simulate the production and propagation of optical photons. There are many detectors which use scintillation and/or Cherenkov photons for their measurements and Geant4 is able to simulate such detectors. Optical photons can be initiated by a charged particle and terminated when entering photo-sensitive areas of the detector. Geant4 provides separate particle definitions for optical photons and gammas, reflecting their very different treatment within a simulation. Refraction and reflection at medium boundaries, bulk absorption, Rayleigh scattering and wavelength shifting processes are provided for optical photons. The optical properties in the medium and at the boundaries are important parameters of these processes. They can be expressed as a function of the photon’s wavelength. However in many cases the user has to supply these parameters by himself. Geant4 provides a framework which assists the user in this.

Photo-lepton_hadron

Geant4 includes photo-nuclear and electro-nuclear reactions in which the energy flow of electrons, positrons and photons is converted into the energy flow of mesons, baryons and nuclear fragments [22]. The cross-section of the photo-nuclear process is comparable with the other electromagnetic processes in the nuclear giant resonance region. The equivalent photon method is applied to the electro-nuclear reactions. Geant4 also provides the nuclear interaction of muons with production of hadrons. This interaction becomes important for the simulation of detector response to high energy muons.

Parameterisation

The processes in this category are used mainly for fast simulations which enable users to take over the tracking of a particle and implement a fast algorithm of detector response. A typical use case is shower parameterisation in a calorimeter. Instead of the detailed simulation of the incident particle which may produce a huge number of secondary particles in the detector, only a few tens of energy deposits will need to be posted in the detector [23,24]. However parameterisations are usually experiment-dependent and/or detector-dependent, so that Geant4 provides only an abstract interface for users.

Hadronic processes of Geant4

The "Russian dolls" (Матрёшка) approach was selected for the hadronic interaction framework in Geant4. It consists of a multi-layer hierarchy, the top level of which provides the basic interface to the other Geant4 categories, such as tracking. As the hierarchy is descended, lower framework levels refine the interfaces for increasingly more specific use cases. Each level except the top has a concrete implementation of the abstract interface from the framework level directory above it, encapsulating the common logic for a particular use-case. The granularity of abstraction and delegation is refined at each framework level in this manner. Through these multi-layered frameworks, code can be developed independently by many users. It also provides significant flexibility to the user. The complete description of all levels of the framework is beyond the aim of this paper and it is given in Ref. [25]. In this paper only the second-level framework is discussed in order to make further explanations intelligible. The components of this level are cross-sections, final state production and isotope production. This level satisfies the requirements that user-defined cross-sections may be added, final state generation and isotope production models may be assigned to processes, and that these components may be used for different parts of the simulation depending on the conditions of the interaction. Thus the hadronic processes of Geant4 can handle multiple cross-section data sets and allow multiple models for final state generation. As a result, the hadronic processes include a large variety of complementary, overlapping and alternative cross-section data sets and physics models.

Physics requirements for the Geant4 hadronic interactions include an energy range which extends from thermal neutrons up to order TeV for LHC experiments and even higher for cosmic ray physics. It extends more than 15 orders of magnitude. In addition to energy range, there is a large variety of particle species and a diversity of interaction types. Geant4 is therefore also required to include the cross-sections of any incident meson or baryon for any materials including long-lived nuclear isotopes. Models of these interactions are also required. The cross-sections and models provided by Geant4 are discussed below.

Geant4 provides the total cross-sections for inelastic scattering, capture of neutral particles, induced fission and elastic scattering for all well known mesons and baryons including ions. The default data-sets for these interactions have been carried over from GEANT3. The term "data-set" represents an object which encapsulates methods and data for computing the occurrence of a given process. It was already mentioned that the software design of Geant4 allows users to overload the default data-sets with their specialised data-sets. The data-sets are stored and retrieved through a data store that works as a First-In-Last-Out stack. In addition to the default data-sets, Geant4 also provides specific data sets for proton- and neutron-induced reactions [26]. For neutron interactions at energies below 20 MeV precise data-sets derived from evaluated neutron data libraries are also available. Later we will discuss these data sets together with the final state generators for these interactions. For ion interactions, in order to cover all combinations of colliding nuclei over a wide energy range with good precision, the cross-section formulae of Tripathi [27,28], Kox [29], Shen [30], and Sihver [31] were implemented in Geant4. These formulae calculate the total reaction cross-section which is the total cross-section minus elastic and electromagnetic dissociation cross-sections. Geant4 also provides data sets for electromagnetic dissociation cross-sections.

The final state modelling methods in the hadronic framework of Geant4 can be classified into three categories: *data-driven*, *parameterised* and *theory-based models*. *Data-driven models* are mainly based on evaluated or measured data. *Parameterised models* are largely based on parameterisations and the extrapolation of experimental data under some theoretical assumptions. *Theory-based models* are predominantly based on theory. In the following, we describe the usage of these modeling approaches in Geant4.

Data-driven models

When experimental or evaluated data are available with sufficient coverage, the data driven approach is considered to be the optimal way of modeling. Neutron High Precision models are typical examples of this category. They are based on the ENDF/B-VI data format and procedures [32] and deal with the detailed transport of neutrons from thermal energies up to 20 MeV. They use the G4NDL neutron data library which is publicly available from the Geant4 web page. This library was derived from the evaluated neutron data libraries Brond-2.1 [33], CENDL2.2 [34], EFF-3 [35], ENDF/B-VI.0 [36], ENDF/B-VI.1, ENDF/BVI.5, FENDL/E2.0 [37], JEF2.2 [38], JENDL-FF [39], JENDL-3.1, JENDL-3.2, and MENDL-2 [40]. Our selection was guided in large part by the FENDL2.0 selection. Enhancement of the libraries is continuing in response to user requests. In these models all inclusive cross-sections are treated as point-wise cross-sections for reasons of performance. For this purpose, the data from the evaluated data library have been processed to explicitly include all neutron nuclear resonances in the form of point-like cross-sections rather than in the form of parameterisations.

The interactions of neutrons at low energies are classified into four parts as are the other hadronic processes in GEANT4. We consider radiative capture, elastic scattering, fission, and inelastic scattering as separate models. The data libraries for high precision neutron models are not complete because there are no data for several key elements in the above cited evaluated neutron data libraries. In order to use the high precision models, users were therefore required to develop their detectors using only elements found in the library. In order to avoid this difficulty, alternative models were developed which use the high precision models when data are found in the library, but use low energy parameterised models (described later) when data are missing. The alternative models cover the same types of interaction as the originals, that is, elastic and inelastic scattering, capture and fission. Because the low energy parameterised part of the models is independent of G4NDL, results will not be as precise as they would be if the relevant data existed. The data driven approach is also used to simulate photon evaporation and radioactive decay. Both codes are based on the ENSDF [41] data of nuclear levels, and transition, conversion, and emission probabilities. The absorption of particles coming to rest and the low energy part of elastic scattering final states in scattering off hydrogen are modelled with this approach.

Parameterised models

Parameterisations and extrapolations of cross-sections and interactions are widely used in the full range of energies and for all kinds of reactions. Low- and high-energy parameterisation models are available in Geant4. They are re-engineered models from GEANT3, predominantly GHEISHA [42]. They include induced fission, capture, elastic and inelastic interactions.

Theory-based models

The models in this category can be divided into three different energy regions such as high energy (above 5 GeV), low energy (below 100 MeV) and intermediate. For high energies, parton string models are used to generate the final state inelastic interactions of hadrons with nuclei in Geant4. Such models can be divided into two phases: string excitation and string fragmentation. Two models which have different approaches to the string excitation phase are implemented. One is based on diffractive excitation and the other so-called Quark Gluon Sting model, is based on soft scattering with diffractive admixture according to cross-sections. In the string fragmentation phase, two models have basically common treatments, but use different fragmentation functions. For intermediate energies intra-nuclear transport models are used. Geant4 provides the Binary Cascade [43] model which is based on a detailed three-dimensional model of the nucleus, and exclusively based on binary scattering between reaction participants and nucleons within the nuclear model, and an implementation of the Bertini Cascade [44]. At energies below 100 MeV exciton-based pre-compound models [45] are provided. They are able to describe the energy and angular distributions of the fast secondaries and soften the behavior of the quasi-elastic peaks to reproduce experimental data.

The last and lowest energy phase of a nuclear interaction is nuclear evaporation. Variants of the classical Weisskopf-Ewing model [46] are used for the interaction. Specialised improvements such as Fermi's break-up model [47] for light nuclei, and multi-fragmentation [48] for very high excitation energies are employed. Fission [49] and photon evaporation including internal conversion can be treated as competitive channels in the evaporation model. A model based on the Generalised Evaporation Model (GEM) [50] is also implemented. For ion interactions the Binary Cascade can handle light ion reactions [51] and Wilson's abrasion model [52] together with its ablation part is also implemented. Electromagnetic dissociation for ion-ion collisions is also treated in Geant4. As an alternative for all nuclear fragmentation models, including evaporation models, the chiral invariant phase space (CHIPS) model [53,54] is available. It is a quark-level 3-dimensional, SU(3) X SU(3) symmetric event generator for fragmentation of excited hadronic and nuclear systems into hadrons. A theoretical model for coherent elastic scattering [55] also exists. This is a hybrid of data-driven and theory-based models, since it utilises a large pre-processed data tabulation.

Other functionalities for shielding calculations

Variance reductions

Variance reduction techniques are an important aspect of most Monte Carlo calculations and allow the user to tune the simulation to the part of the problem space (particle species, energy, position, etc.) most relevant to his/her application [56]. To facilitate the usage of variance reduction techniques, general-purpose biasing methods have been introduced into the toolkit. Many applications, including radiation shielding studies, can profit from this functionality to achieve large gains in time efficiency. A new Geant4 module provides importance biasing, with splitting and Russian roulette [57]; an importance value is associated with each volume. Either the conventional mass geometry (the one used for physics and tracking) or a dedicated artificial parallel geometry can be used for biasing. Other biasing capabilities added in recent releases include an implementation of the weight-window method and of the related, but simpler, weight-cutoff method [58]. Leading particle and cross-section biasing are provided for hadronic processes in the corresponding physics package.

Scoring

Geant4 provides two abstract base classes and one template class for defining detector sensitivity. These classes are flexible and extensible for customisation so that all user requirements may be met. However, users must implement these classes by themselves. Geant4 also offers concrete scoring classes (known as "Primitive Scorer") for common detector sensitivities so that users are not forced to implement their own sensitivities. In this way physical quantities can be obtained more directly and easily.

Conclusion

The Geant4 toolkit provides a full set of software packages for the simulation of particles passing through matter. It adopts an object-oriented design and this implementation allows easy extensions and modifications of the toolkit. Abundant physics processes ranging from thermal neutron interactions in reactor engineering to very high energy interactions in particle physics and cosmic ray physics are provided in the toolkit. It also has variance reduction mechanisms such as importance biasing with weight windows and hands-on user-friendly tallies for simulation results. Therefore, Geant4 already encompasses all aspects of shielding calculations.

All source code and data files of Geant4 is publicly available with documentation from the web. The continuing development of Geant4 is done by the world-wide Geant4 Collaboration.

The scope of Geant4 applications continues to expand.

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