Optical Photon Processes

GEANT4 is an effective and comprehensive tool capable of realistically modeling the optics of scintillation and Cerenkov detectors and their associated light guides. This is founded on GEANT4's unique capacity of commencing the simulation with the propagation of a charged particle and completing it with the detection of the ensuing optical photons on photo sensitive areas, all within the same event loop.

A photon is called 'optical' when its wavelength is much greater than the typical atomic spacing. In GEANT4 the concept of 'optical photons' is a class of particles detached from their higher energy 'gamma' cousins. This implementation allows processes to be associated to them arising from the wave like property of electromagnetic radiation. Since this theoretical description breaks down at higher energies, we are left with the usual conundrum that we don't have a smooth transition as a function of energy between the two types of particles representing the electromagnetic field.

The GEANT4 catalogue of processes at optical wavelengths includes refraction and reflection at medium boundaries, bulk absorption and Rayleigh scattering. The optical properties of the medium which are key to the implementation of these types of processes are stored as entries in a properties table linked to the material in question. They may be expressed as a function of the photon's wavelength. Production of optical photons in a HEP detector is primarily due to the Cerenkov effect and scintillation.

Cerenkov Process

The radiation of Cerenkov light occurs when a charged particle moves through a dispersive medium faster than the group velocity of light in that same medium. Photons are emitted on the surface of a cone; opening at an increasingly acute angle with respect to the particle's momentaneous direction as the particle slows down. At the same time, the frequency of the photons emitted increases and the number produced decreases. When the particle has slowed below the local speed of light, the radiation ceases and the emission cone has collapsed to zero. The photons produced by this process have an inherent polarization perpendicular to the cone's surface at production. The flux, spectrum, polarization and emission of this radiation follow well known formulae in the GEANT4 simulation, albeit with the inherent computational limitation which firstly flows from step wise simulation and secondly, from a numerical integration required to calculate the average number of Cerenkov photons per step.

The need to suspend the primary charged particle track arises in the production of Cerenkov photons because the number of such photons generated during the length of a usual step, as defined by energy loss or multiple scattering, is often very large. Hence, it is common practice to suspend the Cerenkov radiating particle and put it on its own stack of generated secondaries, so that its proteges are tracked in turn before it is revived and transported further.

The time and position of Cerenkov photon emission are calculated from quantities known at the beginning of the charge particle's step, which is assumed to be rectilinear even in the presence of a magnetic field. The user may limit the step size by specifying a maximum average number of Cerenkov photons created during the step. The actual number generated will necessarily be different due to the Poissonian nature of the production.

Scintillation

Every scintillation material has a characteristic light yield and an intrinsic resolution, which generally broadens the statistical distribution due to impurities, which are typical for doped crystals like NaI(Tl) and CsI(Tl). The average yield can have a non-linear dependence on the local energy deposition. Scintillating materials also have emission time spectra with one or more exponential decay time constants, with each decay component having its intrinsic photon emission spectrum. These empirical parameters are typical for each different material and must be supplied by the user. GEANT4 provides a framework in which this can be done effectively.

A Poisson distributed number of photons is generated according to the energy lost during the step and the aforementioned material parameters. The photon's frequency is sampled from empirical spectra. They originate evenly along the track segment and are emitted uniformly with a random linear polarization.

Absorption and Rayleigh Scattering

The implementation of optical photon bulk absorption is trivial in that the process merely 'kills' the particle. The procedure requires the user to fill the relevant material property table with empirical data for the absorption length. Absorption is important because it determines the lower limit in the window of transparency of the radiator.

The differential cross section in Rayleigh scattering is proportional to the square of the cosine of the angle between the new photon's polarization vector and that of the original photon. The Rayleigh scattering process samples this angle accordingly and then calculates the scattered photon's new direction by requiring that it be perpendicular to the photon's new polarization in such a way that the final direction, initial and final polarization are all in one plane. This view compels us to define a (spin) vector representing the photon's precise spin direction. This property is added as a data member to the dynamic particle's description class. A photon which is not conferred a polarization at production may not be Rayleigh scattered.

The Rayleigh process includes a method, which calculates the attenuation coefficient of a medium following the Einstein-Smoluchowski formula whose derivation requires the use of statistical mechanics, includes temperature, and depends on the isothermal compressibility of the medium. This method is convenient when the Rayleigh attenuation length is not known from measurement but may be calculated from first principles using the above material constants. Rayleigh scattering is usually unimportant except for large

water Cerenkov detectors for neutrino detection and aerogel, which is used as a Cerenkov radiator for some special applications.

Reflection and Refraction

To explain the simulation of reflection and refraction at medium boundaries, two preliminary remarks are necessary about navigation and the concept of surfaces.

Navigation at Medium Boundaries

When a track exits a volume, the navigator class in GEANT4 stores an exit normal to the volume surface pointing outwards if the track leaves the volume completely. If the track enters a daughter volume, no exit normal is available and the boundary process has to invoke a public method of the navigator class explicitly to calculate the surface normal, as well as transformation methods for the normal vector from local to global coordinates and vice versa. Comparing the final volume's mother pointer with the original volume's pointer is used to identify the two situations.

The boundary process is a 'discrete process' as defined by GEANT4 convention and is therefore called at the end of a particle's step, but unlike other such processes, the boundary process never limits the step; transportation does this already. In turn, its process implementation is called at every step by always setting the 'forced' condition. Hence, the code must first verify that the track is really at a boundary before springing into action. Similarly, upon reflection the GEANT4 navigator makes a zero length step and since the boundary process is always invoked, it has to be able to identify this situation as well. In this way, the process establishes that as a consequence of the logic of the GEANT4 navigator, the previous step was a 'null' step and consequently, reflection has just taken place, and although still at the boundary, no further action should be taken. With other words, the boundary process implementation is rigid about what it expects the GEANT4 navigator does upon reflection on a boundary.

Surface Concept

The optical boundary process design relies heavily on the concept of 'surfaces'. The information is split into two classes. One class in the materials category keeps information about the physical properties of the surface itself, and a second class in the geometry category holds pointers to the relevant physical or logical volumes involved and has an association to the physical class. The second type of surface objects are stored in a related table and can be retrieved by either specifying the two ordered pair of physical volumes touching at the surface, or by the logical volume entirely surrounded by this surface. The former is called a 'border surface' while the latter is referred to as a 'skin' surface. This second type of surface is useful in situations where a volume is coded with a reflector and is placed into many different mother volumes. A limitation is that the skin surface can only have one and the same optical property for all of the enclosed volume's sides. The 'border surface' is an ordered pair of physical volumes, so in principle, the user can choose different optical properties for photons arriving from

reverse sides of the same interface. Optical boundary processes are at present only possible for volumes that have been position by using placement rather than replica or touchables.

The physical surface object also specifies which model the boundary process should use to simulate interactions with that surface. In addition, the physical surface can have a material property table all its own. The usage of this table allows all specular constants to be wavelength dependent. In case the surface is painted, wrapped or has a cladding, the table may include the thin layer's index of refraction. This allows the simulation of boundary effects both at the intersection between the medium and the surface layer, as well as at the far side of the thin layer, all within the process itself and without invoking the GEANT4 navigator. Combinations of surface finish properties, such as polished or ground and front painted or back painted, enumerate the different situations.

Implementation

Optical boundary processes are distinguished in that they are not local and the actual physics, which happens at the interface, depends on the material beyond the boundary. The source of the problem is the particle description of what is essentially a wave phenomenon. The evanescent wave in the less dense medium during total internal reflection is a striking example. The solution for the purpose of simulation relies on the recognition that processes do not have to be confined to a single step, and that the actual execution (DoIt) of the physics process may be deferred until all relevant information for the process is available. In this scheme an optical photon will always penetrate, i.e. be stepped into the new medium before a decision is made between refraction and reflection.

When a photon arrives at a medium boundary its behaviour depends on the nature of the two materials that join at that boundary. The medium boundary may be specified as between two dielectric materials, one dielectric and a metal, or one dielectric and a 'black' medium. In the case of two dielectric materials the photon can be total internal reflected, refracted or reflected, depending on the photon's wavelength, angle of incidence, (linear) polarization and the refractive indices on both sides of the boundary. The photon can be absorbed by the metal or reflected back into the dielectric. If the photon is absorbed it can be detected according to the photoelectron efficiency of the metal. Reflection and transmission probabilities are sensitive to the state of linear polarization.

Inasmuch as Fresnel reflection and refraction are intertwined through their relative probabilities of occurrence, as expressed in Maxwell's equations, neither process, nor total internal reflection, are viewed as individual processes deserving separate class implementation. Nonetheless, we tried to adhere to the abstraction of having independent processes by splitting the code into different methods where practicable.

One implementation of the boundary process employs the UNIFIED model [reference] of the DETECT [reference] program. The original GEANT3 implementation of this process is also available via the GLISUR methods flag. The UNFIED model tries to provide a

realistic simulation that deals with all aspects of surface finish and reflector coating. The surface may be assumed as smooth and covered with a metal coating representing a specular reflector with given reflection coefficient, or painted with a diffuse reflecting material where Lambertian reflection occurs. The surfaces may or may not be in optical contact with another component and most importantly, one may consider a surface to be made up of micro-facets with normal vectors that follow given distributions around the nominal normal for the volume at the impact point. For very rough surfaces, it is possible for the photon to inversely aim at the same surface again after reflection or refraction and so multiple interactions with the boundary are possible within the process itself and without the need for relocation by the GEANT4 navigator.

The UNIFIED model provides for a range of different reflection mechanisms. The specular lobe constant represents the reflection probability about the normal of a micro facet. The specular spike constant, in turn, illustrates the probability of reflection about the average surface normal. The diffuse lobe constant is for the probability of internal Lambertian reflection, and finally the back scatter spike constant for the case of several reflections within a deep grove with the ultimate result of exact back scattering.