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Technical Notes

Simulating response functions and pulse shape discrimination for organic scintillation detectors with Geant4

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ABSTRACT

We present new capabilities of the Geant4 toolkit that enable the precision simulation of organic scintillation detectors within a comprehensive Monte Carlo code for the first time. As of version 10.0-beta, the Geant4 toolkit models the data-driven photon production from any user-defined scintillator, photon transportation through arbitrarily complex detector geometries, and time-resolved photon detection at the light readout device. By fully specifying the optical properties and geometrical configuration of the detector, the user can simulate response functions, photon transit times, and pulse shape discrimination. These capabilities enable detector simulation within a larger experimental environment as well as computationally evaluating novel scintillators, detector geometry, and light readout configurations. We demonstrate agreement of Geant4 with the NRESP7 code and with experiments for the spectroscopy of neutrons and gammas in the ranges 0–20 MeV and 0.511–1.274 MeV, respectively, using EJ301-based organic scintillation detectors. We also show agreement between Geant4 and experimental modeling of the particle-dependent detector pulses that enable simulated pulse shape discrimination.

1. Introduction

The simulation of organic scintillation detectors in neutron and gamma fields has long been of interest to the detector physics community for two primary reasons. First, simulation helps interpret the complex detector response functions that are generated by the nonlinear production of scintillation photons as a function of energy deposited and ionizing particle type. Second, simulation can easily generate a large number of detector response functions for various incident particles, which can be difficult to obtain experimentally. These response functions are required as inputs to unfolding codes that deconvolve the incident particle energy spectrum from the detector response. In addition, simulation can play an important role in the computational design and optimization of new types of particle detectors that are based on organic scintillators.

In this paper, we present the implementation and validation of new organic scintillation detector modeling capabilities contained in the Geant4 toolkit as of version 10.0-beta. The method enables the user to fully simulate time-resolved production (linear or nonlinear), transport, and readout of photons in a detector of arbitrary geometry, scintillator choice, structural materials, and light readout configuration, all potentially within the complexity of an encompassing experiment geometry. This is the first time that such comprehensive detector modeling can be performed within a single Monte Carlo (MC) code, leading to significant improvements in the simulation of detector response in complex environments and the optimization of advanced design for scintillation detectors.

This paper is structured as follows: Section 2 describes the motivation behind this work; Section 3 overviews the simulation capabilities of Geant4 for organic scintillators; Section 4 describes the hardware used to experimentally validate Geant4 for organic scintillation detectors; Section 5 demonstrates Geant4's ability to correctly simulate organic scintillation detector response functions for incident neutrons (0–20 MeV) and gammas (0.511–1.274 MeV); and Section 6 demonstrates Geant4's ability to correctly simulate the timing properties of individual scintillator light pulses, which enables the simulation of pulse shape discrimination.

2. Motivation

The most widely used configuration for organic scintillation detectors is a right cylinder scintillator coupled to a photomultiplier tube (PMT) of similar size to optimize light collection. However, new scintillator materials, such as pulse shape discriminating plastic [1] and new light readout devices, such as silicon photomultipliers

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(SiPMs), can now be used to fabricate detectors in a wide variety of complex geometries, materials, and light readout configurations. For these "advanced" organic scintillation detectors, the capability to perform high fidelity modeling of the detector response functions and pulse shape discrimination (PSD) would greatly enhance computational detector design.

Existing codes are not well suited to such work. Although used successfully for decades to model organic scintillation detectors, previous codes such as SCINFUL [2] and NRESP7 [3] are limited to right cylinder geometries, provide limited particle sources, do not model the light readout device, and restrict the simulation boundary to the detector itself. Recently, codes such as MCNP-PoliMi [4] and MCNPX-PHOTRACK [5] have extended somewhat the detector complexity and simulation domain that can be modeled but require significant post processing and code coupling. Although MCNPX-PHOTRACK can estimate the effect of optical parameters on PSD, neither code can directly simulate PSD via the time-resolved production, transport, and detection of optical photons.

One of the principal motivations for this work was to develop a single MC code that could comprehensively model the optical physics of advanced organic scintillation detectors. This can play an important role in guiding detector design and optimization. A second motivation was the desire to include this capability within the framework of a general purpose MC code – Geant4 in particular – in order to calculate detector response functions within a larger simulated experiment. This is crucial for a Geant4-based simulation of a new type of particle accelerator-based instrument, which studies the evolution of materials inside magnetic confinement fusion reactors [6].

3. Geant4

Geant4 is an object-oriented C++ Monte Carlo toolkit for simulating the passage of particles through matter [7]. Most aspects of simulating EJ301-based scintillation detectors with Geant4 have been extensively studied [8–12].

All of these studies, however, neglect the production, transportation, and detection of scintillation photons, choosing to score the energy deposition in the scintillator volume and then apply scintillation response and detector resolution functions to replicate the full experimental detector response. While successful in many applications, this approach is not ideal as it obscures the influence of optical properties on the detector response, requires substantial knowledge of the scintillator light response and detector energy resolution, necessitates post-processing work by the user to generate detector response functions, and is not applicable to computationally exploring complex detector geometries or nonstandard light readouts.

As of Geant4.10.0-beta (released June 2013), a new model for energy- and particle-dependent scintillation, coupled to the pre-existing optical physics capabilities, enables the user to simulate an organic scintillation detector of arbitrary complexity with a minimum amount of overhead. We briefly describe the new scintillation model and optical transport capabilities of Geant4 below; for detailed description and instruction on implementing these features in user simulations, the reader is referred to Section 5.2.5 of the Geant4 User's Guide for Application Developers [13].

3.1. Scintillation model

In Geant4, as in all other MC codes, a continuous particle trajectory is necessarily broken into many small steps in order to correctly simulate the passage of the particle through matter, which has important implications for simulating the scintillation light response. In scintillators with a linear response, light production is directly proportional to the ionizing energy deposited in the scintillator. Thus, the total light produced along a particle track in the scintillator can be computed as the sum of the light produced in smaller steps without regard for the kinetic energy of the ionizing particle at each energy-depositing step.

In scintillators with a nonlinear response, the light produced in each step must be computed as

$$L_{\text{step}} = L(T, x) - L(T - E_{\text{dep}}, x) \tag{1}$$

where L is the number of scintillation photons, T is the kinetic energy of the charged particle before the step, E_{dep} is the total ionizing energy deposited in the scintillator during the step, and x is the charged particle type depositing energy. In addition to correctly modeling the total light produced by a multiple step ionizing particle track in a scintillator, this methodology accounts for two important cases. First, light is produced correctly for incomplete energy deposition of the charged particle, such as is the case where the particle exits the scintillator volume ("wall effects") or in the case that the particle is absorbed in a nuclear reaction. Second, the scintillation photon density is larger in the high-kinetic energy portion of the ionizing particle track in the usual case where the nonlinear photon yield increases with particle energy.

3.2. Optical physics models

In Geant4, optical photons are linearly transported in media with an imputed index of refraction, until they are either bulk absorbed, are Mie or Rayleigh scattered, or encounter a medium boundary. The boundary can be between two dielectric materials or a dielectric and a metal. In the latter case, the photons can be reflected or absorbed, in which case absorbed photons can be deemed detected after sampling a user-specified wavelength dependent detection efficiency.

The UNIFIED model [14], originally developed for the DETECT MC program [15] provides a range of different reflection mechanisms (specular lobe, specular spike, Lambertian and back-scatter spike) and polished and rough optical surfaces. A simpler roughness model, GLISUR [16], carried over from an earlier version of Geant(3) is also available. For an entirely empirical surface model, the results of measurements of the angular reflectivity distribution inside of a BGO crystal, for combinations of common surface treatments and different applied reflectors, are available in look-up-tables (LUTs) [17].

A scintillator material is characterized by its photon emission spectrum, its rise time, and its exponential decay time components. Two time decay components are possible with defined relative strength, and they can have different emission spectra. A characteristic light yield is part of the scintillator's material definition, with the actual simulated number statistically sampled around this mean. When the scintillation yield is a non-linear function of the energy deposited and varies between particle types, an array of total scintillation light yields as a function of deposited energy may be defined for protons, electrons, deuterons, tritons, alphas, and carbon ions, enabling precision modeling of any scintillator's light response.

4. Experimental setup

This sections describes the hardware setup – particle detectors and data acquisition system – used to experimentally validate the capability of Geant4 to simulate organic scintillation detectors.