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NUCLEIDE++: A C++ MODULE TO INCLUDE DDEP RECOMMENDED RADIOACTIVE DECAY DATA IN GEANT4

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ABSTRACT

In ionizing radiation metrology, radionuclide nuclear decay scheme data are crucial, in particular to determine detection efficiency by means of algorithms, e.g. in gamma spectrometry and liquid scintillation counting (LSC) or in physical models used in Monte Carlo codes. The NUCLEIDE database provides comprehensive and accurate data recommended by the Decay Data Evaluation Project (DDEP), well suited to metrological applications. Few years ago, a FORTRAN subroutine PENNUC, which simulates random decay pathways of a radionuclide using the NUCLEIDE database, was developed by CIEMAT in collaboration with LNE-LNHB. This algorithm can be used either independently to generate a list of emitted particles, or directly in the PENELOPE Monte Carlo code.

Following this previous work, an equivalent tool NUCLEIDE++, written in C++, and designed to work in conjunction with the GEANT4 Monte Carlo toolkit has been developed. The module simulates the complete decay scheme for a given radionuclide by randomly selecting the decay pathways, using data from NUCLEIDE: half-life, nuclear level structure for the parent and daughter nuclide, branching ratios, type and energy of emitted particles. The nuclear de-excitation of the potential daughters can also be treated in the same run. The initial energies of the electron and positron in the case of beta-emitting radionuclides are sampled from spectra calculated with the BetaShape program developed at LNE-LNHB. The de-excitation cascade, i.e. the set of transitions that occur from an initial vacancy, is sampled from the transition probabilities provided in the Lawrence Livermore National Laboratory (LLNL) Evaluated Atomic Data Library (EADL), according to the KLM atomic re-arrangement models.

The aim of this work is to propose to GEANT4 users the possibility to run with the recommended NUCLEIDE data and a more detailed model, as an alternative to the current radioactive decay module in which the simulation model depends on data taken from the Evaluated Nuclear Structure Data File (ENSDF). The reliability of NUCLEIDE++ is shown by comparing the coincident particles cascades to the ones obtained with PENNUC and GEANT4, in the case of some radionuclides with complex decay schemes (^{152}Eu, ^{133}Ba,^{166m}Ho,^{113}Sn), and beta-emitting radionuclides for which the precision of the beta spectrum has been determined at LNE-LNHB (^{63}Ni, ^{241}Pu, ^{60}Co). Multi-gamma spectra simulated with NUCLEIDE++ are also compared with measurements.

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