Educational project

Basics of simulation with Geant4-DNA extension: Applications in quantitative radiation biology

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1. Description of the project

The initial physical structure of high-energy heavy-charged (HZE) particle tracks plays an important role in understanding the basic mechanism of radiation actions on biological tissues. Charged particle track-structure simulations are a useful tool for the interpretation and understanding of early physical and chemical stages of radiation actions on matter. These Monte-Carlo based simulations provide detailed information on properties of the interactions such as spatial distribution of energy depositions, interaction types (ionization, excitation, elastic scattering, charge change, etc.), and radical species produced. Geant4-DNA is in progress to extend the Geant4 simulation toolkit to model the effects of radiation with biological systems at cellular and DNA level.

This practical course will instruct attendees in use of Geant4-DNA process at different level, applicable for computational radiation biology [1, 2] and any application fields. The course will include material and hands-on exercises on microdosimetry calculation methods, developing own codes describing the target geometry, tracking and physical processes, 3D reconstruction of the DNA atomistic model [3] and simulation of radioactive isotope decays at nanometer scale [4].

2. Goal of the project

The aim of proposed practical work is to gain an experience of students in applications of microdosimetry calculation method. In particular, it is focused on better understanding initial radiation effects of HZE particles at DNA scale: quantitative estimation of DNA damages on reconstructed 3D model of DNA molecules under exposure to HZE particles.

3. Short description of the exercises

1. Simulation of physical interactions of HZE particles with biological media (liquid water and DNA molecules).
2. Developing of own codes describing the target geometry, tracking and physical processes using on the microdosimetry calculation methods.
3. 3D reconstruction of the DNA atomistic model from available experimental data bases.
4. Obtaining and analyzing of the simulation results.

4. Enter requirements

1. Basic knowledge of the physics of ionizing radiation interaction with matter and biological tissues.
2. Little prior experience of Linux operating systems and Geant4 Monte-Carlo toolkit/ C++ programming language. At least theoretical knowledge about analysis of data with ROOT software, Wolfram Mathematica or Origin.
5. Example screenshots of particle track structures in biological media

Figure 1. (a) An example of 1 MeV $^4$He ion track structure (LET = 103 keV/µm) simulated by Geant4-DNA inside the ellipsoid target of 3×4×6 nm$^3$ liquid water. (b) The spectrum of the energy deposition in the target volume.

Figure 2. Atomistic models of the 12 base pair B-DNA (a) and 146 base pair nucleosome (b) exposed to 1 MeV/u $^4$He ion track simulated with Geant4-DNA. The coordinates of the native DNA and nucleosome geometry are obtained from Protein Data Bank (PDB).

Figure 3. The radioactive decay (a) and energy deposition along the radius (b) from Iodine-125 radioisotope inside a cell nucleus at the DNA scale. The different low energy electromagnetic process of Geant4-DNA and Geant4-Livermore are used.

6. The number of participating students is limited to 2.

7. References

8. Contacts of the project coordinators
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