Educational project

Geant4 Applications in Computational Radiation Biology

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1. Description of the project

Understanding the fundamental mechanisms involved in the induction of biological damage by ionizing radiation remains a major challenge of today's radiobiology research. The initial track-structure simulations of high-energy heavy-charged (HZE) particles are a useful tool for the interpretation and plays an important role in 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 free radical species produced. Geant4 is a powerful tool for the simulation of the passage of radiation through matter, and it can be used in a wide range of applications: from space applications to microdosimetry and medical applications [1]. This practical course will instruct attendees in use of Geant4-DNA extension of the general purpose Monte Carlo Geant4 simulation toolkit for modeling of the early effects of radiation with biological systems at cellular and DNA level [2]. The course will include several hands-on exercises on microdosimetry calculation methods: developing own codes describing the target geometry with different materials, tracking and physical/chemical processes, 3D modeling of the DNA atomistic structure and estimation of direct and indirect DNA damages.

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 (basic) radiation effects of HZE particles at DNA scale; depth and radial dose distributions of different LET (linear energy transfers) particles; quantitative estimation of base and both strands DNA damages under irradiation with HZE particles.

3. Short description of the exercises

1. Track structure simulation of physical, physico-chemical and chemical 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. Modeling of the DNA and nucleosomes atomistic structures from available experimental data bases (PDB).
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. An example screenshots of particle track structures in biological media

a)

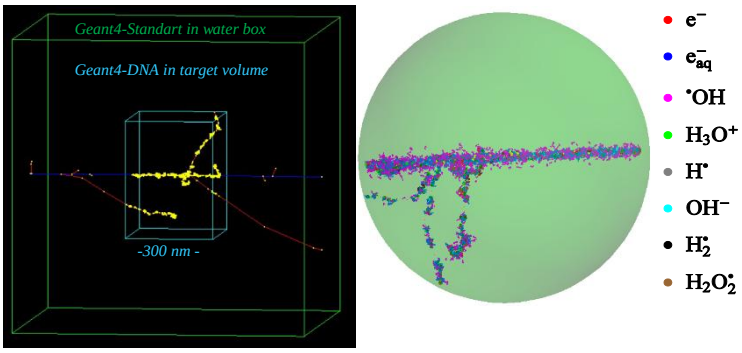
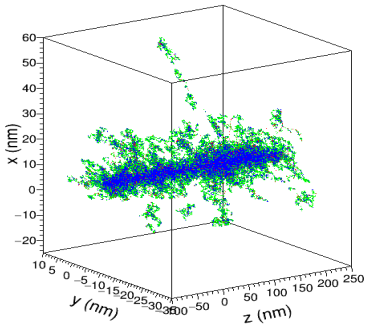


Figure 1. An example of 1 MeV/u ^{4}He ion track structure segment (LET = 103 keV/μm) generated by Geant4-Standart and Geant4-DNA physics processes inside the water box and target of 300 nm of liquid water (left). The water radiolysis of ^{4}He particle inside sphere solid with radius of 300 nm (right).



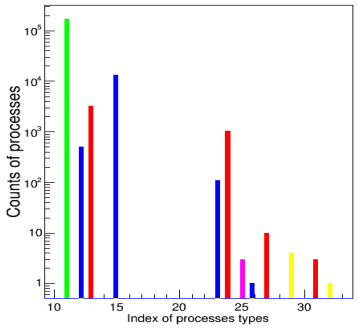
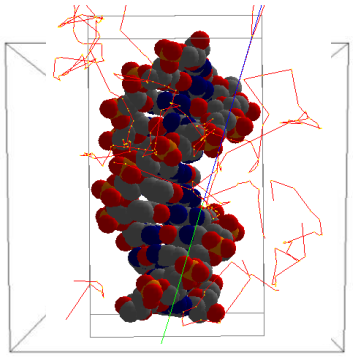


Figure 2. The ionization (red), excitation (blue), elastic scattering(green), dissociative electron attachment (yellow), charge decrease (magenta) and charge increase (cyan) physical processes in ^{4}He ion track segment (left, in nm of scale) and total amount of their physics processes (right).



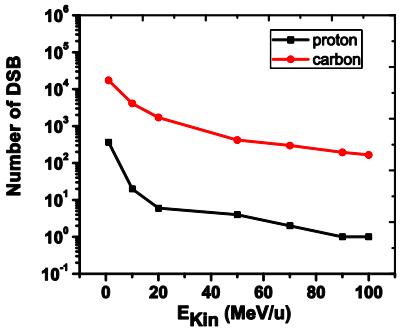


Figure 3. Atomistic models of the 12 base pair B-DNA exposed to 1 MeV/u ^{4}He ion track simulated with Geant4 (left). Yields of double strand breaks (DBS) after irradiation with different particles as a function of the particles kinetic energies (right).

6. The number of participating students is limited to 4.

7. References

1. GEANT4 HOME PAGE and http://geant4-dna.org/ .
2. M. Batmunkh, L. Bayarchimeg, O. Lkhagva, O. Belov, Cluster Analysis of HZE Particle Tracks as Applied to Space Radiobiology Problems, // Physics of Particles and Nuclei Letters (Springer). (2013); Vol. 10. №. 7 (184), P. 854-859.

8. Contacts of the project coordinator

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