Overview of the Geant4-DNA software for early DNA damage prediction

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Synopsis Modeling accurately early biological damage induced by ionizing radiation at the scale of the DNA molecule remains a major challenge of today's radiobiology research. In order to provide the community with an easily accessible mechanistic simulation platform, the general-purpose and open-source "Geant4" Monte Carlo simulation toolkit is being extended in the framework of the "Geant4-DNA" project with a set of functionalities allowing the detailed simulation of particle-matter interactions in biological medium. We will present an overview of the Geant4-DNA project and discuss on-going developments.

The Geant4-DNA Collaboration [1] is extending the general-purpose and open-source Geant4 particle-matter simulation toolkit [2] for radiobiology applications. Initially developed for the simulation of high energy physics experiments (eg. ATLAS and CMS that revealed the Higgs boson in 2012) at the European Organization for Nuclear Research (CERN, Switzerland), Geant4 is being extended with specific functionnalities, including [3-6] :

- Several sets of physics processes describing the dominant discrete physical interactions of electrons, protons, hydrogen atoms, alpha particles and their charged states in liquid water, the main component of biological medium. These can be combined with existing Geant4 processes for the description of other processes, such as photon interactions.

- Physico-chemistry and chemistry processes which can simulate water radiolysis from physical interactions, that is the creation, the diffusion and mutual reactions of molecular species in liquid water, up to 1 microsecond after irradiation.

- Detailed geometries of biological targets: benefiting from Geant4 geometry modeling capabilities, it is now possible to simulate geometries of biological targets, such as the DNA molecule up to cell nuclei and neural networks. An illustration is shown in Fig. 1 for the implementation a simplified geometrical model of *E. coli* bacterium genome.

These developments can be combined in order to predict early DNA damage. In particular, on-going developments allow the prediction of indirect damage in bacteria and cells and pave the way to the inclusion of repair mechanisms, extending simulation capabilities well beyond the microsecond.

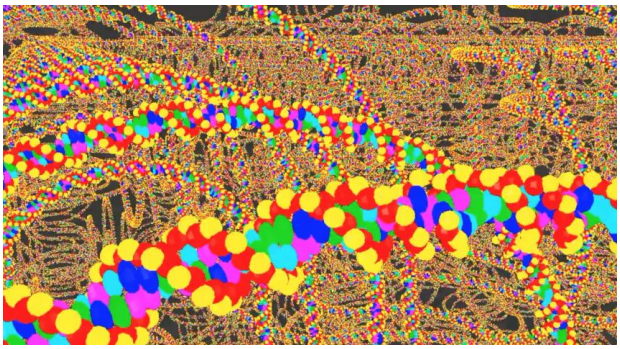

Figure 1. Geant4-DNA geometrical modeling of E. coli bacterium genome.

All features described above are fully accessible through the Geant4 simulation toolkit and can be run using our freely downloadable Linux™ CentOS™ virtual machine [7]. We hope that this platform and its future developments will be useful for the further mechanistic understanding of ionizing radiation effects in biological targets, especially when high spatial resolution (nanometer) and low energy (few electonsVolts) simulations are required.

References

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