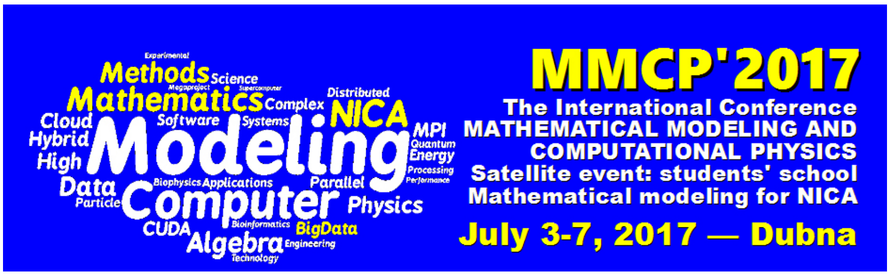

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Monte Carlo simulation of early biological damage induced by ionizing radiation at the DNA scale: overview of the Geant4-DNA project

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INTRODUCTION

Modeling accurately biological damage induced by ionizing radiation at the scale of the DNA molecule remains a major challenge of today's radiobiology research (1). In order to provide the community with an easily accessible mechanistic simulation platform, the general purpose and open source "Geant4"Monte Carlo simulation toolkit (2) is being extended in the framework of the "Geant4-DNA"project (3) with a set of functionalities allowing the detailed simulation of particle-matter interactions in biological medium. These functionalities include physical, physico-chemical and chemical processes that can be combined with nanometer size geometries of biological targets in order to predict early DNA damage. We will present an overview of the Geant4-DNA project and discuss on-going developments.

THE GEANT4-DNA EXTENSION OF GEANT4

The main developments undertaken by the Geant4-DNA collaboration (3-5) cover three main areas:
• Physics processes: several sets of physics processes are available in order to describe 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: such processes 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 accurate geometries of biological targets, such as the DNA molecule.

These developments can be combined in order to predict early DNA damage. In particular, on-going developments will lead to 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.

OUTCOME

All features described above are fully accessible (6) through the Geant4 simulation toolkit and can be run using a freely downloadable Linux (TM) CentOS (TM) 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.

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