DNA-sequenced geometrical modelling in GEANT4-DNA

R. Khanna[1], Y. Reinwald[1], G.A.P. Cirrone[2], S. Fattori[2,3], A. Serjouei[1]

[1]Department of Engineering, School of Science and Technology, Nottingham Trent University, Nottingham, UK
[2]Istituto Nazionale di Fisica Nucleare, Laboratori Nazionali del Sud, Catania, Italy
[3]ENEA - Centro Ricerche Casaccia Via Anguillarese, Rome, Italy

Background: GEANT4-DNA provides several examples to simulate biological damages induced by ionizing radiation at the cellular and sub-cellular levels. To date, several new biological geometries have been modelled. This includes several different cells and their optimisation, for example, including the euchromatin and hetrochromatin densities in the model, sub-cellular structure's such as the plasmid and chromatin fibre and geometries obtained from confocal microscopy[1–3]. These works have focused mainly on the positioning and compaction of genetic material in a nucleus rather than the specific content of the genetic material.

Material and Methods: Based on the wholeNuclearDNA example in GEANT4-DNA, accurate base pair DNA sequencing is used to model different genes at the chromatin fibre level. The sequenced DNA is looped around histones to create a nucleosome which is positioned to create a chromatin fibre.

Preliminary results: The assessment from corrections and advances in DNA modelling, as shown in Figure 1, and biological events at the gene expression stage enabled reliable evaluation of biological damage from ionising radiation.

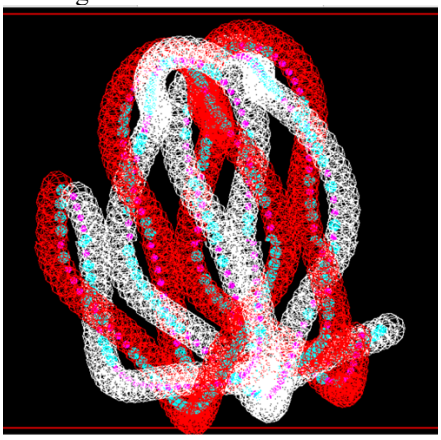

Figure 1: Simulation of 200 DNA base pairs sequenced specific to the Col1a1 gene present in a fibroblast cell used in the geometry of the chromatin fibre of the gene.

(1) Thibaut, Y. *et al.* Isochore Nuclear Geometry for Modeling the Radiation-Induced DNA Damage Toplogy. *ERRS 2021*.
(2) D-Kondo, N. *et al.* DNA Damage Modeled with Geant4-DNA: Effects of Plasmid DNA Conformation and Experimental Conditions. *Phys. Med. Biol.* **2021**, *66* (24), 245017.
(3) Gonon, G. *et al.* From Energy Deposition of Ionizing Radiation to Cell Damage Signaling: Benchmarking Simulations by Measured Yields of Initial DNA Damage after Ion Microbeam Irradiation. *Radiat. Res.* **2019**, *191* (6), 566–584.