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”molecularDNA” example application for the simulation of radiation-induced DNA damage using Geant4-DNA

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A significant effort is underway in the global scientific community to develop accurate models of DNA damage in cells induced by hadronic particles, in the context of hadrontherapy cancer treatment or for future manned space exploration missions. Several Monte Carlo Track Structure software codes (MCTS) have been developed for simulating early-DNA scale events to macroscopic radiobiological endpoints. These include cell survival, single and double DNA breaks, DNA repair, and other late effects. The Geant4-DNA extension (https://geant4-dna.org/) of the Geant4 (GEometry ANd Tracking) toolkit is the first open-source and general-purpose MCTS code, delivering a framework for simulating the physical interaction of radiation with DNA molecules and the chemical stages of water radiolysis, including the production of oxidative radical species. It also provides a variety of geometrical models of cell nuclei with a complete DNA genome implemented. The geometries of cell nuclei are, by default, seeded from a fractal packing, where the DNA chain is a continuous Hilbert curve made of straight and turned chromatin sections, including nucleosomes. A new model of cell nuclei, named “complexDNA,” has been recently created, incorporating all 23 chromosome pairs of a human cell. It shows minimal discrepancies in DNA damage yield compared to the default model and achieves around three times improved CPU time. The geometric models are interfaced with the direct and indirect stages of DNA damage induction, and the advanced example of Geant4-DNA named “molecularDNA” was released in December 2022 (https://moleculardna.org). An overview of the “molecularDNA”application will be provided, covering its design, purpose, and key features, and will include a demonstration of its predictive performance compared to experimental data from helium ion beam irradiation of cancer cells. DNA rejoining and cell survival prediction in V79 cells using Geant4-DNA will also be presented. The new computational approach for generating complex chromosomal DNA geometries will be described along with a discussion of other methods to enhance the modelling of cell geometries.

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Primary author: DORDEVIC, Milos (Vinca Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University of Belgrade, Mike Petrovica Alasa 12-14, 11351 Vinca, Belgrade, Serbia)

Co-authors: Prof. CHATZIPAPAS, Konstantinos (Reactor Institute Delft, Department of Radiation Science & Technology, Delft University of Technology, 2629 JB Delft, Netherlands); Dr TRAN, Hoang Ngoc (University of Bordeaux, CNRS, LP2I Bordeaux, UMR 5797, Gradignan, F-33170, France); Dr SAKATA, Dousatsu (Division of Health

Sciences, The University of Osaka, Osaka 565-0871, Japan); Dr MUNKHBAATAR, Batmunkh (Laboratory of Radiation Biology, JINR, Dubna 141980, Russia); Dr KETA, Otilija (Vinca Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University of Belgrade, Mike Petrovica Alasa 12-14, 11351 Vinca, Belgrade, Serbia); Dr PETKOVIC, Vladana (Vinca Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University of Belgrade, Mike Petrovica Alasa 12-14, 11351 Vinca, Belgrade, Serbia); Dr INCERTI, Sebastien (University of Bordeaux, CNRS, LP2I Bordeaux, UMR 5797, Gradignan, F-33170, France)

Presenter: DORDEVIC, Milos (Vinca Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University of Belgrade, Mike Petrovica Alasa 12-14, 11351 Vinca, Belgrade, Serbia)

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