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Development of an optimised method for tracking chemical species in Geant4-DNA enabling in-silico radiobiology in a cosmic radiation environment

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Modelling the early DNA damage induced by radiation is critical for understanding its biological impact. Radiation traversing a cell induces DNA damage through both physical interactions (direct damage) and chemical interactions of radiochemical species (indirect damage) with the DNA strand. Through the combination of DNA geometry models, physics models and chemical tracking, the early DNA damage in a cell can be simulated in silico using the Geant4-DNA toolkit. However, there are great computational requirements for the simulation of high linear energy transfer (LET) particles because of the great number of chemical species requiring simultaneous tracking.

In this study, a new chemical species tracking model was developed to improve the computational efficiency of the chemical tracking. This was achieved by applying the Synchronous Independent Reaction Time model in different spatial segments simultaneously. This led to an improvement in execution time by over an order of magnitude for particles with an LET beyond ~ 10 keV/um. This model allows the chemical process to be distributed over multiple computer cores, leading to an improvement in computational resource utilisation.

The new chemical tracking model was validated using radiobiological experiments undertaken at ANSTO. 149BR human skin fibroblasts were irradiated with protons and carbon ions having the same energy per mass unit of 3 MeV/u. The cells were stained for γ -H2AX foci, which represent the location of double strand breaks (DSBs). Confocal imaging was used to obtain the three-dimensional foci distribution. These were compared with simulated γ -H2AX foci images using Geant4-DNA, demonstrating the ability of Geant4-DNA to predict radiobiological effects of radiation.

Author: ARCHER, Jay (University of Wollongong)

Co-authors: Dr SAKATA, Dousatsu (National Institute of Advanced Industrial Science (AIST)); Dr TRAN, Hoang (University of Bordeaux); Dr BROWN, Jeremy (Swinburne University); ROUGHLEY, Kiarn (University of Wollongong); FERLAZZO, Melanie (Australian Nuclear Science and Technology Organisation (ANSTO)); Dr TEHEL, Moeava (University of Wollongong); Dr DRURY, Ryan (Australian Nuclear Science and Technology Organisation (ANSTO)); Dr INCERTI, Sebastien (University of Bordeaux); Dr PERACCHI, Stefania (Australian Nuclear Science and Technology Organisation (ANSTO)); GUATELLI, Susanna; Dr PASTUOVIC, Zeljko (Australian Nuclear Science and Technology Organisation (ANSTO))

Presenter: GUATELLI, Susanna

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