DNA damage simulation and prediction of biological endpoints using Geant4-DNA - Development of molecularDNA -

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Background: Track structure Monte Carlo (MC) codes (such as KURBUC, PARTRAC, and Geant4-DNA) have achieved successful outcomes in the quantitative investigation of radiation-induced initial DNA damage. We developed a fully integrated Geant4-DNA application called “molecularDNA” which allow the simulation of early DNA damage induced after irradiation at DNA/Cell level and prediction of biological endpoints (typically cell survival), aiming at investigation of radiobiological phenomena. In this presentation, we introduce “molecularDNA” including its development history, and how we can predict the biological endpoints using the application.

Material and Methods: We developed an application “molecularDNA”. The development of the application body was described in the publications [1-3] and the extensions for prediction of subsequent biological endpoints were described [4-6], as well. Moreover, additional validations were presented [7,8].

Preliminary results: “molecularDNA” is able to simulate successfully the early DNA damage after irradiation and its complexity. Using this application, it is possible to predict radiobiological endpoints such as accumulation of repair proteins, DNA rejoining kinetics, and cell survival (Figure 1.). The application has been released in Geant4 version 11 BETA (July 2022).

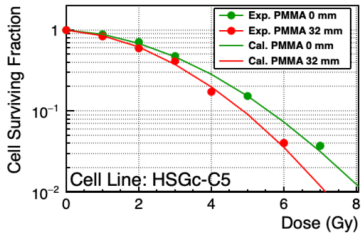

Figure 1: cell survival of HSGc-C5 cells after proton irradiation.

[1] N. Lampe *et al.* Phys. Med. 48, 135-145 (2018)
[2] N. Lampe *et al.* Phys. Med. 48, 146-155 (2018)
[3] D. Sakata *et al.* Phys. Med. 62, 152-157 (2019)
[4] D. Sakata *et al.* Sci. Rep. 10, 20788 (2020)
[5] D. Sakata *et al.* Phys. Med. Under Review
[6] D. Sakata *et al.* Cancers 13(23), 6046 (2021)
[7] W.-G. Shin *et al.* Cancers 13(19), 4940 (2021)
[8] K. Chatzipapas *et al.* Prec. Radiat. Oncle. Under Review